

## CURRICULUM VITAE

### Alexander M. Mebel

**Education:**            *Undergraduate* (B.Sc., Physical Chemistry)  
University: Moscow Institute of Steel and Alloys (1984)  
*Graduate* (Ph.D., Physical Chemistry)  
Kurnakov's Institute of General and Inorganic Chemistry  
Russian Academy of Science, Moscow, Russia (1990)

#### **Professional Experience:**

8/24-current	<u>Chair</u> Department of Chemistry and Biochemistry Florida International University, Miami, Florida
8/14-current	<u>Professor</u> Department of Chemistry and Biochemistry Florida International University, Miami, Florida
8/10-8/14	<u>Professor and Graduate Program Director</u> Department of Chemistry and Biochemistry Florida International University, Miami, Florida
8/07-8/10	<u>Associate Professor</u> Department of Chemistry and Biochemistry Florida International University, Miami, Florida
8/03-8/07	<u>Assistant Professor</u> Department of Chemistry and Biochemistry Florida International University, Miami, Florida
10/01-8/03	<u>Associate Research Fellow</u> Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan
7/98-9/01	<u>Assistant Research Fellow</u> Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan
2/98-6/2000	<u>Visiting Assistant Professor</u> Tamkang University, Tamsui, Taiwan
1/96-6/98	<u>Senior Academia Sinica Postdoctoral Fellow</u> Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan
10/93-12/95	<u>Senior Research Associate</u> Chemistry Department, Emory University, Atlanta, Georgia, USA
8/92-9/93	<u>Visiting scientist, special researcher</u> Institute for Molecular Science, Okazaki, Japan.
9/91-3/92	<u>Visiting researcher</u> Institut für Organische Chemie Universität Erlangen-Nürnberg, Erlangen, Germany
6/87-2/93	<u>Research worker</u>
7/84-5/87	<u>Engineer</u> Laboratory of Quantum Chemistry Institute of New Chemical Problems Russian Academy of Science in Chernogolovka, Moscow, Russia
9/89-5/91	<u>Lecturer</u> All-Union Polytechnic Institute Moscow, Russia

## Awards

Academia Sinica Research Award for Junior Researches	2002
IAMS Outstanding Publication Award	2003
Florida International University CASE Research Award	2016
Florida International University CASE Service Award	2018
FIU Faculty Convocation Award for Excellence in Research	2019
Fellow of The Combustion Institute	2021
Florida International University CASE Research Award	2021
39 <sup>th</sup> International Combustion Symposium Distinguished Paper Award	2023
40 <sup>th</sup> International Combustion Symposium Distinguished Paper Award	2025

## Research, Professional, and Mentorship Experience

Dr. Mebel's research area is applications-oriented theoretical chemistry, i.e., computer simulations of the behavior of molecules based on 'the first principles' – the laws of quantum mechanics. He uses theoretical calculations to investigate chemical and photochemical reactions relevant to combustion of fossil fuels, atmospheric chemistry, astrochemistry, material science, organometallic complexes in aqueous and organic solutions, and other chemical fields. The theoretical studies involve state-of-the-art quantum chemical methods using modern computer clusters and represent a valuable tool for characterization and prediction of various physico-chemical and spectroscopic properties of molecules and their reactivity and for interpretation of experimental data. These studies provide highly accurate and reliable data on the geometric and electronic structure, relative energies of reaction intermediates and products, and barrier heights involved in various reaction mechanisms. He graduated six Ph.D. students and provided mentorship to numerous undergraduate students.

## Publications

(646 publications and 15,836 citations on Web of Science as of July 2024, 12,960 excluding self-citations, SCI h-index 60)

## Regular Articles

1. Mebel A.M., Zyubina T.S.  
Nonempirical calculations of the potential surface and molecular structure of aluminum oxide ( $\text{Al}_2\text{O}$ ) in singlet and triplet states.  
Zh. Neorg. Khim. 1987, 32, 1285-1289.
2. Mebel A.M., Klimenko N.M., Charkin O.P.  
Structure and stability of the lithiated  $\text{ALi}_k$  and  $\text{ALi}_{k+1}^+$  clusters of the 2nd and 3rd period elements by non-empirical calculations with electronic correlation taken into account.  
Zh. Strukt. Khim. 1988, 29, 12-21.
3. Klimenko N.M., Mebel A.M., Charkin O.P.  
Peculiarity of electronic structure of the hypovalent  $\text{ALi}_k$  and  $\text{ALi}_{k+1}^+$  lithides.  
Zh. Strukt. Khim. 1988, 29, 22-27.
4. Korokin A.A., Mebel A.M., Borisov E.V.  
Nonempirical study of the isomers of the PNO oxyphosphonitride.  
Izvestia of USSR Acad. Sci., 1988, 900-903.

5. Korkin A.A., Mebel A.M., Tsvetkov E.N.  
Theoretical study of the effect of protonation on the phosphorus-nitrogen bond of amino phosphines.  
Zh. Obshch. Khim., 1988, 58, 1015-1021.
6. Mebel A.M., Charkin O.P., Kuznetsov I.Yu., Solntsev K.A., Kuznetsov N.T.  
Theoretical study of structure and migration non-rigidity of the  $B_6H_7^-$  and  $LiB_6H_7$  closoboranes.  
Zh. Neorg. Khim., 1988, 33, 1685-1689.
7. Mebel A.M., Charkin O.P., Solntsev K.A., Kuznetsov N.T.  
Theoretical study of structure and migration non-rigidity of the  $B_{10}H_{11}^-$  closoborane anion.  
Zh. Neorg. Khim., 1988, 33, 2263-2269.
8. Mebel A.M., Charkin O.P.  
Theoretical study of the reaction of the  $H_2$  molecule cleavage from the  $B_6H_7^-$  anion.  
Zh. Neorg. Khim., 1989, 34, 275-280.
9. Mebel A.M., Charkin O.P., Solntsev K.A., Kuznetsov N.T.  
Theoretical study of structure and migration non-rigidity of the  $B_7H_8^-$  and  $B_8H_9^-$  anions.  
Zh. Neorg. Khim., 1989, 34, 281-289.
10. Mebel A.M., Charkin O.P.  
Theoretical study of structure and stability of fluoro-substituted derivatives of the closoborane  $B_6F_iH_{6-i}^{2-}$  anion.  
Zh. Neorg. Khim., 1989, 34, 611-617.
11. Mebel A.M., Charkin O.P.  
Theoretical study of migration non-rigidity of the closoborane salts  $Li_2B_6H_6$ ,  $BeB_6H_6$ ,  $(BeH)_2B_6H_6$ , and  $LiB_6H_6^-$ .  
Zh. Strukt. Khim., 1989, 30, 7-18.
12. Mebel A.M., Charkin O.P., Solntsev K.A., Kuznetsov N.T.  
Theoretical study of structure and migration non-rigidity of the  $B_9H_{10}^-$  anion.  
Zh. Neorg. Khim., 1989, 34, 1435-1443.
13. Mebel A.M., Charkin O.P., Solntsev K.A., Kuznetsov N.T.  
Theoretical study of structure and migration non-rigidity of the  $B_{12}H_{13}^-$  anion.  
Zh. Neorg. Khim., 1989, 34, 1444-1448.
14. Musaev D.G., Mebel A.M., Chimiraglia R., Tomasi J., Charkin O.P.

Nonempirical study of isomerization in the CuAlO and CuCP molecules by pseudopotential method.

- Koord. Khim., 1989, 15, 1155-1161.
15. Yakobson V.V., Musaev D.G., Zyubin A.S., Mebel A.M., Charkin O.P.  
Theoretical study of  $\text{Li}^+$  affinity of the hydrides  $\text{MH}_n$ , fluorides  $\text{MF}_n$ , and lithides  $\text{MLi}_n$  molecules.  
Koord. Khim., 1989, 15, 1478-1488.
  16. Mebel A.M., Charkin O.P.  
Theoretical study of structure of the  $\text{AlB}_5\text{H}_6^{2-}$ ,  $\text{CB}_5\text{H}_6$ ,  $\text{SiB}_5\text{H}_6^-$  anions and their protonated derivatives  $\text{AlB}_5\text{H}_7^-$ ,  $\text{CB}_5\text{H}_7$ , and  $\text{SiB}_5\text{H}_7$ .  
Zh. Neorg. Khim., 1990, 35, 312-319.
  17. Korkin A.A., Mebel A.M.  
Comparative nonempirical study of the conjugation effects in iminophosphines and iminophosphoranes.  
Metalorg. Khim., 1990, 3, 1005-1011.
  18. Mebel A.M., Charkin O.P., Klimenko N.M.  
Theoretical study of the hexalithide clusters  $\text{ALi}_6$ .  
Zh. Neorg. Khim., 1991, 36, 439-450.
  19. Mebel A.M., Charkin O.P., Klimenko N.M.  
Theoretical study of structure and stability of beryllium hydride clusters  $(\text{BeH})_k$  ( $k = 2, 4, 6$ ),  $\text{A}(\text{BeH})_4$ , and  $\text{A}(\text{BeH})_6$ .  
Zh. Neorg. Khim., 1991, 36, 741-751.
  20. Mebel A.M., Charkin O.P.  
Theoretical study of reactions of molecular hydrogen with active centers in the  $\text{B}_6\text{H}_5^-$  and  $\text{AlB}_5\text{H}_5^-$  clusters.  
Zh. Neorg. Khim., 1991, 36, 2354-2367.
  21. Mebel A.M., Charkin O.P.  
Nonempirical study of potential surface of the least motion path of  $\text{AlH} + \text{H}_2 \rightarrow \text{AlH}_3$  reaction.  
Zh. Neorg. Khim., 1991, 36, 2368-2375.
  22. Mebel A.M., Charkin O.P.  
Theoretical study of reactions of molecular hydrogen with active centers in the  $\text{CB}_5\text{H}_5$  and  $\text{SiB}_5\text{H}_5$  clusters.  
Zh. Neorg. Khim., 1991, 36, 2881-2888.
  23. Solntsev K.A., Mebel A.M., Votnova N.A., Kuznetsov N.T., Charkin O.P.  
Polyhedral anion  $\text{B}_{12}\text{H}_{12}^{2-}$  as three-dimensional aromatic system.  
Koord. Khim., 1992, 18, 340-364.
  24. Buehl M., Mebel A.M., Charkin O.P., Schleyer P.v.R.

- The structure of  $B_8H_8^{2-}$  in solution. Is  $B_8H_9^-$  also involved? An ab initio/IGLO/NMR study.  
Inorg. Chem., 1992, 31, 3769-3775.
25. Mebel A.M., Charkin O.P.  
Theoretical of reactions of molecular hydrogen with active centers in the  $B_nH_{n-1}^-$  clusters.  
Zh. Neorg. Khim., 1992, 37, 2355-2362.
  26. Mebel A.M., Strunina E.V., Charkin O.P.  
Theoretical study of reactions of cluster active center insertion into the C-H and C-C bonds.  
Zh. Neorg. Khim., 1992, 37, 2363-2374.
  27. Borisov E.V., Mebel A.M., Knyazev B.A., Zabrodin V.B., Korokin A.A.  
Comparative nonempirical study and isodesmic calculations of heats of formation of HNCO and HPCI isomers.  
Izvestia of Russ. Acad. Sci., Ser. Khim. 1992, 41, 1585-1590.
  28. Mebel A.M., Charkin O.P., Buehl M., Schleyer P. v. R.  
The structure and non-rigidity of  $B_{10}H_{11}^-$ . Ab initio/IGLO/NMR study.  
Inorg. Chem., 1993, 32, 463-468.
  29. Mebel A.M., Charkin O.P., Schleyer P. v. R.  
Theoretical prediction of the structure and non-rigidity of  $B_7H_8^-$ . Application of the ab initio/IGLO/NMR method.  
Inorg. Chem., 1993, 32, 469-473.
  30. Mebel A.M., Musaev D.G., Morokuma K.  
Ab initio MO study of mechanisms of the reaction of  $B_2H_6$  with  $SH_2$ .  
J. Phys. Chem. 1993, 97, 7543-7552.
  31. Mebel A.M., Musaev D.G., Morokuma K.  
Ab initio molecular orbital study of structure and NMR  $^{11}B$  chemical shifts of Lewis base adducts of CO,  $NH_3$ ,  $PF_3$ , and  $PH_3$  with small nido-boranes,  $B_3H_7$  and  $B_4H_8$ .  
Chem. Phys. Lett. 1993, 214, 69-76.
  32. Mebel A.M., Musaev D.G., Koga N., Morokuma K.  
Metallaboranes with 8 and 9 group transition metals. Is accurate ab initio molecular orbital calculation of structure, stability and NMR  $^{11}B$  chemical shifts possible?  
Bull. Chem. Soc. Jpn. 1993, 66, 3259-3270.
  33. Mebel A.M., Musaev D.G., Morokuma K.

- An alternative mechanism of BH<sub>2</sub>SH formation in the reaction of B<sub>2</sub>H<sub>6</sub> with SH<sub>2</sub>: Concerted elimination of BH<sub>3</sub> and H<sub>2</sub> from H<sub>2</sub>S·B<sub>2</sub>H<sub>6</sub>. Ab initio MO study.  
Chem. Phys. Lett. 1993, 216, 313-318.
34. Mebel A.M., Morokuma K., Musaev D.G.  
Ab initio MO study of cluster rearrangements in pentagonal pyramidal clusters, B<sub>6</sub>H<sub>10</sub> borane and [(IrB<sub>5</sub>H<sub>8</sub>)(CO)(PH<sub>3</sub>)<sub>2</sub>] metallaborane.  
J. Am. Chem. Soc., 1994, 116, 3932-3942.
  35. Mebel A.M., Morokuma K., Lin M.C.  
Ab Initio Molecular Orbital Study of Potential Energy Surface for the NH+NO<sub>2</sub> Reaction.  
J. Chem. Phys., 1994, 101, 3916-3922.
  36. Herges R., Mebel A.M.  
Propargylene.  
J. Am. Chem. Soc., 1994, 116, 8229-8237.
  37. Mebel A.M., Lin M.C.  
Ab initio molecular orbital calculations of C<sub>6</sub>H<sub>5</sub>O<sub>2</sub> isomers.  
J. Am. Chem. Soc., 1994, 116, 9577-9584.
  38. Musaev D.G., Mebel A.M., Morokuma K.  
An ab initio molecular orbital study of the mechanism of the rhodium(I)-catalyzed olefin hydroboration reaction.  
J. Am. Chem. Soc., 1994, 116, 10693-10702.
  39. Yu T., Mebel A.M., Lin M.C.  
The reaction of phenoxy radical with nitric oxide.  
J. Phys. Org. Chem., 1995, 8, 47-53.
  40. Musaev D.G., Matsubara T., Mebel A.M., Koga N., Morokuma K.  
Ab initio molecular orbital studies of elementary reactions and homogeneous catalytic cycles with organometallic compounds.  
Pure Appl. Chem., 1995, 67, 257-263.
  41. Mebel A.M., Morokuma K., Lin M.C., Melius C.F.  
Potential energy surface of the HNO+NO reaction. An ab initio molecular orbital study.  
J. Phys. Chem., 1995, 99, 1900-1908.
  42. Mebel A.M., Isobe K., Morokuma K.  
A theoretical study of rectangular tetrasulfur in a gas phase and in the tetranuclear [{Rh<sub>2</sub>(η<sup>5</sup>-C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>(μ-CH<sub>2</sub>)<sub>2</sub>]<sub>2</sub>(μ-S<sub>4</sub>)]<sup>2+</sup> complex.  
Inorg. Chem., 1995, 34, 1208-1211.
  43. Lin M.C., Mebel A.M.  
An ab initio molecular orbital study of the O + C<sub>6</sub>H<sub>5</sub>O reaction.  
J. Phys. Org. Chem., 1995, 8, 407-420.

44. Mebel A.M., Lin M.C., Morokuma K., Melius C.F.  
Theoretical study of the gas phase structure, thermochemistry and decomposition mechanisms of  $\text{NH}_4\text{NO}_2$  and  $\text{NH}_4\text{N}(\text{NO}_2)_2$ .  
J. Phys. Chem., 1995, 99, 6842-6848.
45. Mebel A.M., Morokuma K., Lin M.C.  
Ab initio molecular orbital study of potential energy surface for the reaction of  $\text{C}_2\text{H}_3$  with  $\text{H}_2$  and related reactions.  
J. Chem. Phys., 1995, 103, 3440-3449.
46. Mebel A.M., Hsu, C.-C., Lin M.C., Morokuma K.  
An ab initio molecular orbital study of potential energy surface of the  $\text{NH}_2 + \text{NO}_2$  reaction.  
J. Chem. Phys., 1995, 103, 5640-5649.
47. Mebel A.M., Morokuma K., Lin M.C.  
Modification of the GAUSSIAN-2 theoretical model: The use of coupled-cluster energies, density-functional geometries, and frequencies.  
J. Chem. Phys., 1995, 103, 7414-7421.
48. Mebel A.M., Morokuma K.  
Theoretical Study of the Reaction of  $\text{HCl}$  with  $\text{ClONO}_2$  catalyzed by  $\text{NO}_3^-$ . "Attachment-Detachment" Mechanism for the Anion-Catalyzed Neutral Reactions.  
J. Phys. Chem., 1996, 100, 2985-2992.
49. Mebel A.M., Lin M.C., Morokuma K., Melius C.F.  
Theoretical rate constants for the  $\text{NH}_3 + \text{NO}_x \rightarrow \text{NH}_2 + \text{HNO}_x$  ( $x = 1, 2$ ) reactions by ab initio MO/VTST calculations.  
J. Phys. Chem., 1996, 100, 7517-7525.
50. Liu R., Morokuma K., Mebel A.M., Lin M.C.  
Ab initio study of the mechanism for the thermal decomposition of the phenoxy radical.  
J. Phys. Chem., 1996, 100, 9314-9322.
51. Mebel A.M., Chen Y.-T., Lin S.H.  
 $\pi$ - $\pi^*$  vibronic spectrum of ethylene from ab initio calculations of the Franck-Condon factors.  
Chem. Phys. Lett., 1996, 258, 53-62.
52. Hsu C.-C., Mebel A.M., Lin M.C.  
Ab initio molecular orbital study of the  $\text{HCO} + \text{O}_2$  reaction: direct vs. indirect abstraction channels.  
J. Chem. Phys., 1996, 105, 2346-2352.
53. Luna A., Mebel A.M., Morokuma K.  
A molecular orbital study of the global potential energy surfaces

- of the [H,C,N,O]<sup>+</sup> system in doublet and quartet states.  
J. Chem. Phys., 1996, 105, 3187-3205.
54. Mebel A.M., Lin M.C., Morokuma K., Melius C.F.  
Theoretical study of reactions of N<sub>2</sub>O with NO and OH radicals.  
Int. J. Chem. Kinet., 1996, 28, 693-703.
55. Mebel A.M., Luna A., Lin M.C., Morokuma K.  
Theoretical study of the global potential energy surfaces of the [H,C,N,O]  
system  
in singlet and triplet states.  
J. Chem. Phys., 1996, 105, 6439-6454.
56. Mebel A. M., Diau E. W. G., Lin M. C., Morokuma K.  
Ab Initio and RRKM Calculations for Multichannel Rate Constants of the  
C<sub>2</sub>H<sub>3</sub> + O<sub>2</sub> Reaction.  
J. Am. Chem. Soc., 1996, 118, 9759-9771.
57. Mebel A.M., Chen Y.-T., Lin S.H.  
On the theoretical investigation of vibronic spectrum of ethylene by ab initio  
calculations of the Franck-Condon factors.  
J. Chem. Phys., 1996, 105, 9007-9020.
58. Madden L.K., Mebel A.M., Lin M.C., Melius C.F.  
A theoretical study of the thermal isomerization of fulvene to benzene.  
J. Phys. Org. Chem., 1996, 9, 801-810.
59. Moskaleva L.V., Mebel A.M., Lin M.C.  
The CH<sub>3</sub> + C<sub>5</sub>H<sub>5</sub> reaction: a potential source of benzene at high  
temperatures.  
Twenty Sixth Symposium (International) on Combustion, The Combustion  
Institute: Pittsburgh, 1996, pp. 521-526.
60. Halbgewachs M.J., Diau E.W.G., Mebel A.M., Lin M.C., Melius C.F.  
Thermal reduction of NO by NH<sub>3</sub>: kinetic modeling of the NH<sub>2</sub> + NO product  
branching ratio.  
Twenty Sixth Symposium (International) on Combustion, The Combustion  
Institute: Pittsburgh, 1996, pp. 2109-2116.
61. Hsu C.-C., Lin M.C., Mebel A.M., Melius C.F.  
Ab initio study of the H + HONO reaction: direct abstraction versus indirect  
exchange processes.  
J. Phys. Chem. A, 1997, 101, 60-66.
62. Mebel A.M., Lin S.H., Chang C.-H.  
Theoretical study of vibronic spectra and photodissociation pathways of  
methane.  
J. Chem. Phys., 1997, 106, 2612-2620.
63. Mebel A.M., Lin S.H.

Excited Electronic States of the Methyl Radical. Ab Initio Molecular Orbital Study of Geometries, Excitation Energies and Vibronic Spectra. Chem. Phys., 1997, 215, 329-341.

64. Mebel A.M., Lin M.C., Yu T., Morokuma K.  
Theoretical study of potential energy surface and thermal rate constants for  $C_6H_5 + H_2$  and  $C_6H_6 + H$  reactions.  
J. Phys. Chem. A, 1997, 101, 3189-3196.
65. Hayashi M., Yang T.S., Mebel A.M., Chang C.H., Lin S.H., N.F. Scherer  
Vibronic and vibrational coherence and relaxation dynamics of molecules in condensed phases.  
Chem. Phys., 1997, 217, 259-273.
66. Richardson S.L., Francisco J.S., Mebel A.M., Morokuma K.  
Can chlorine anion catalyze the reaction of HOCl with HCl.  
Chem. Phys. Lett., 1997, 270, 395-398.
67. Hayashi M., Yang T.S., Yu J., Mebel A.M., Lin S.H.  
Spectroscopy and ultrafast dynamics in the electron donor-acceptor complex: TCNE-HMB.  
J. Phys. Chem. A, 1997, 101, 4156-4162.
68. Mebel A.M., Hayashi M., Lin S.H.  
Ab Initio Calculations of Vibronic Coupling. Applications to Symmetry-Forbidden Vibronic Spectra and Internal Conversion in Ethylene  
Chem. Phys. Lett., 1997, 274, 281-292.
69. Mebel A.M., Chen Y.-T., Lin S.H.  
Ab initio molecular orbital study of excited electronic states of the vinyl radical.  
Chem. Phys. Lett., 1997, 275, 19-27.
70. Park J., Dyakov I.V., Mebel A.M., Lin M.C.  
Experimental and Theoretical Studies of the Unimolecular Decomposition of Nitrosobenzene: High-Pressure Rate Constants and the C-N Bond Strength  
J. Phys. Chem. A, 1997, 101, 6043-6047.
71. Jackson W.M., Mebel A. M., Lin S. H., Lee Y. T.  
Using ab initio MO calculations to understand the photodissociation dynamics of  $CH_2CCH_2$  and  $CH_2C_2$   
J. Phys. Chem. A, 1997, 101, 6638-6646.
72. Mebel A. M., Lin S. H., Yang X. M., Lee Y. T.  
Theoretical Study on the Mechanism of the Dissociation of Benzene. The  $C_5H_3 + CH_3$  Product Channel.  
J. Phys. Chem. A, 1997, 101, 6781-6789.
73. Wang Y.-L., Mebel A.M., Wu C.-J., Chen Y.-T., Lin C.-E., Jiang J.-C.

Infrared spectroscopic observation and theoretical vibrational calculation of melamine molecule.

- J. Chem. Soc., Faraday Trans., 1997, 93, 3445-3451.
74. Liao D.-W., Mebel A.M., Chen Y.-T., Lin S.H.  
A Theoretical Study of the Structure, Energetics and the  $n-\pi^*$  electronic transition of the acetone +  $n\text{H}_2\text{O}$  ( $n=1-3$ ) complexes.  
J. Phys. Chem. A, 1997, 101, 9925-9934.
75. Mebel A.M., Lin M.C.  
Theoretical studies of reactions of  $\text{NO}_x$  with nitrogen hydrides.  
Int. Rev. Phys. Chem., 1997, 16, 249-266.
76. Hayashi M., Mebel A.M., Liang K.K., Lin S.H.  
Internal conversion rate constant for polyatomic molecules. Ab initio study of radiationless transitions between excited and ground singlet electronic states of ethylene.  
J. Chem. Phys., 1998, 108, 2044-2055.
77. Mebel A.M., Lin M.C., Melius C.F.  
Rate constant of the  $\text{HONO} + \text{HONO} \rightarrow \text{H}_2\text{O} + \text{NO} + \text{NO}_2$  reaction from ab initio MO and TST calculations.  
J. Phys. Chem., 1998, 102, 1803-1807.
78. Mebel A.M., Schleyer P.v.R., Charkin O.P., Najafian K.  
The structure and nonrigidity of  $\text{B}_9\text{H}_9^{2-}$  and  $\text{B}_9\text{H}_{10}^-$ . Comparisons of  $\text{B}_n\text{H}_{n+1}^-$  systems.  
Inorg. Chem., 1998, 37, 1693-1703.
79. Mebel A.M., Lin S.H., Pinnaduwa L.A.  
Potential energy surfaces of excited states of  $\text{H}_2^-$ .  
Chem. Phys. Lett., 1998, 285, 114-120.
80. Chang A.H.H., Mebel A.M., Yang X.-M., Lin S.H., Lee Y.T.  
Ab Initio Calculations of Potential Energy Surface and Rate Constants for Ethylene Photodissociation at 193 and 157 nm  
Chem. Phys. Lett., 1998, 287, 301-306.
81. Mebel A.M., Jackson W.M., Chang A.H.H., Lin S.H.  
Photodissociation dynamics of propyne and allene: a view from ab initio calculations of the  $\text{C}_3\text{H}_n$  ( $n = 1-4$ ) species and the isomerization mechanism of  $\text{C}_3\text{H}_2$ .  
J. Am. Chem. Soc., 1998, 120, 5751-5763.
82. Hayashi M., Yang T.-S., Yu J., Mebel A.M., Chang R., Lin S.H., Rubtsov I.V., Yoshihara K.  
Vibronic and vibrational coherence and relaxation dynamics in the TCNE-HMB complex  
J. Phys. Chem. A, 1998, 102, 4256-4265.
83. Chang A.H.H., Mebel A.M., Yang X.-M., Lin S.H., Lee Y.T.

- Ab initio/RRKM approach toward the understanding of ethylene photodissociation  
 J. Chem. Phys., 1998, 109, 2748-2761.
84. Mebel A.M., Lin M.C., Morokuma K.  
 Ab initio MO and TST calculations for the rate constant of the  $\text{HNO} + \text{NO}_2 \rightarrow \text{HONO} + \text{NO}$  reaction.  
 Int. J. Chem. Kinet., 1998, 30, 729-736.
  85. Hwang D.-Y., Mebel A.M.  
 Ab initio study on the reaction mechanism of ozone with chlorine atom  
 J. Chem. Phys., 1998, 109, 10847-10852.
  86. Schleyer P.v.R., Najafian K., Mebel A.M.  
 The large closo-borane dianions,  $\text{B}_n\text{H}_n^{2-}$  ( $n = 13-17$ ) are aromatic, why are they unknown?  
 Inorg. Chem., 1998, 37, 6765-6772.
  87. Ju S.-S., Han C.-C., Wu C.-J., Mebel A. M., Chen Y.-T.  
 The fragmentation of melamine: A study via electron-impact ionization, laser-desorption ionization and collision-induced dissociation, and density functional calculations of potential energy surface for various dissociation channels.  
 J. Phys. Chem. B, 1999, 103, 582-596.
  88. Mebel A.M., Lin H.L, Lin S.H.  
 Ab Initio Molecular Orbital and Density Functional Study of the  $\text{C}_6\text{H}_6 \cdot \text{I}_2$  Complex in the Ground and Excited Electronic States  
 Int. J. Quantum Chem., 1999, 72, 307-318.
  89. Mebel A.M., Najafian K., Charkin O.P., Schleyer P.v.R.  
 An ab initio study of protonation of  $\text{B}_{12}\text{H}_{12}^{2-}$ . Structure and nonrigidity of  $\text{B}_{12}\text{H}_{13}^-$  and formation of  $\text{B}_{12}\text{H}_{11}^-$  and  $\text{B}_{24}\text{H}_{23}^{3-}$   
 J. Mol. Struct. (THEOCHEM), 1999, 461-462, 187-202.
  90. Mebel A.M., Moskaleva L.V., Lin M.C.  
 Ab initio MO calculations for the reactions of  $\text{NH}_2$  with  $\text{H}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{NH}_3$ , and  $\text{CH}_4$ : prediction of absolute rate constants and kinetic isotope effects  
 J. Mol. Struct. (THEOCHEM), 1999, 461-462, 223-238.
  91. Mebel A.M., Lin M.C.  
 Prediction of absolute rate constants for the reactions of  $\text{NH}_2$  with alkanes from ab initio G2M/TST calculations  
 J. Phys. Chem. A, 1999, 103, 2088-2096.
  92. Pinnaduwege L.A. , Ding W.X., McCorkle D. L., Lin S.H., Mebel A.M., Garscadden A.  
 Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges  
 J. Appl. Phys., 1999, 85, 7064-7069.

93. Kaiser R.I., Mebel A.M., Chang A.H.H., Lin S.H., Lee Y.T.  
Crossed-beam reaction of carbon atoms with hydrocarbon molecules V:  
Chemical dynamics of n-C<sub>4</sub>H<sub>3</sub> formation from reaction of C(<sup>3</sup>P<sub>j</sub>) with allene,  
H<sub>2</sub>CCCH<sub>2</sub> (X<sup>1</sup>A<sub>1</sub>)  
J. Chem. Phys., 1999, 110, 10330-10344.
94. Chang A.H.H., Hwang D.W., Yang X.-M., Mebel A.M., Lin S.H., Lee Y.T.  
Toward understanding of ethylene photodissociation: theoretical study of  
energy partition in products and rate constants  
J. Chem. Phys., 1999, 110, 10810-10820.
95. Liao D.-W., Mebel A.M., Hayashi M., Shiu Y.J., Chen Y.-T., Lin S.H.  
Ab initio study of the n-π\* electronic transition in acetone: symmetry-forbidden  
vibronic spectra  
J. Chem. Phys., 1999, 111, 205-215.
96. Hwang D.-Y., Mebel A.M., Wang B.C.  
Ab initio study of the addition of atomic carbon with water  
Chem. Phys., 1999, 244, 143-149.
97. Mebel A.M., Hayashi M., Liang K.K., Lin S.H.  
Ab initio calculations of vibronic spectra and dynamics for small polyatomic  
molecules: The role of Duschinsky Effect (Feature Article)  
J. Phys. Chem. A, 1999, 103, 10674-10690.
98. Hayashi M., Liang K.K., Chang C.H., Mebel A.M., Lin S.H.  
Recent developments in radiationless transitions  
Journal of Photoscience, 1999, 6, 97-102.
99. Mebel A.M., Lai M.Y., Wang Y.L.  
Two-dimensional Ga-induced magic clusters on the Si surface: a density  
functional study  
Chem. Phys. Lett., 2000, 318, 27-34.
100. Mebel A.M., Kaiser R.I., Lee Y.T.  
Ab initio MO study of the global potential energy surface of C<sub>4</sub>H<sub>4</sub> in triplet  
electronic state and the reactions of C(<sup>3</sup>P<sub>j</sub>) with C<sub>3</sub>H<sub>4</sub> (allene and propyne)  
and C<sub>2</sub>(a<sup>3</sup>Π<sub>u</sub>) with C<sub>2</sub>H<sub>4</sub>(X<sup>1</sup>A<sub>1g</sub><sup>+</sup>)  
J. Am. Chem. Soc., 2000, 122, 1776-1788.
101. Hwang D.-Y., Mebel A.M.  
Theoretical study on the reversible storage of H<sub>2</sub> by BeO  
Chem. Phys. Lett., 2000, 321, 95-100.
102. Shieh J.-C., Chang J.-L., Wu, J.-C., Li R., Mebel A.M., Handy N.C., Chen Y.-  
T.

Rydberg states of propyne at 6.8-10.5 eV studied by two-photon spectroscopy  
and theoretical calculation

- J. Chem. Phys., 2000, 112, 7384-7393.
103. Hwang D-Y., Mebel A.M.  
Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide  
Chem. Phys., 2000, 256, 169-176.
  104. Zyubin A.S., Mebel A.M., Lin S.H.  
Ab initio study of H photodetachment from the ethyl radical  
Chem. Phys. Lett., 2000, 323, 441-447.
  105. Mebel A.M., Baer M., Lin S.H.  
Probing the Nature of Surface Intersection by Ab Initio Calculations of Non-Adiabatic Coupling Matrix Elements: Conical Intersection due to Bending Motion in C<sub>2</sub>H  
J. Chem. Phys., 2000, 112, 10703-10706.
  106. Hwang D-Y., Mebel A.M.  
Theoretical Study on Reforming of CO<sub>2</sub> Catalyzed with Be  
Chem. Phys. Lett., 2000, 325, 639-644.
  107. Nguyen T.L., Le T.N., Mebel A.M., Lin S.H.  
Heats of formation of small bicyclic hydrocarbons, spiro[3.3]heptane (C<sub>5</sub>H<sub>8</sub>), spiro[3.4]heptane (C<sub>5</sub>H<sub>8</sub>) and bicyclo[1.1.0]but-1(3)-ene (C<sub>4</sub>H<sub>4</sub>): a theoretical study by the G2M(RCC,MP2) method  
Chem. Phys. Lett., 2000, 326, 468-476.
  108. Hwang D-Y., Mebel A.M.  
Theoretical Study on Reaction Mechanism of CO<sub>2</sub> with Mg  
J. Phys. Chem. A, 2000, 104, 7646-7650.
  109. Hwang D-Y., Mebel A.M.  
Ab initio study of the reaction mechanism of singlet and triplet N<sub>2</sub>O and their intersystem crossing  
Chem. Phys., 2000, 259, 89-97.
  110. I. Handorf, H. Y. Lee, A. M. Mebel, S. H. Lin, Y. T. Lee, R. I. Kaiser  
A combined crossed beam and ab initio investigation on the reaction of carbon species with C<sub>4</sub>H<sub>6</sub> isomers I: The 1,3-butadiene molecule, H<sub>2</sub>CCHCHCH<sub>2</sub> (X<sup>1</sup>A')  
J. Chem. Phys., 2000, 113, 9622-9636.
  111. L. C. L. Huang, H. Y. Lee, A. M. Mebel, S. H. Lin, Y. T. Lee, R. I. Kaiser  
A combined crossed beam and ab initio investigation on the reaction of carbon species with C<sub>4</sub>H<sub>6</sub> isomers II: The dimethylacetylene molecule, H<sub>3</sub>CCCCH<sub>3</sub> (X<sup>1</sup>A<sub>1g</sub>)  
J. Chem. Phys., 2000, 113, 9637-9648.
  112. Hwang D-Y., Mebel A.M.  
Theoretical study on the reversible storage of H<sub>2</sub> by BeS

- J. Am. Chem. Soc., 2000, 122, 11406-11410.
113. Hwang D-Y., Mebel A.M.  
Reaction mechanism of CO<sub>2</sub> with Ca atom: A theoretical study  
Chem. Phys. Lett., 2000, 331, 526-532.
  114. Mebel A.M., Hwang D-Y.  
Theoretical Study on Reaction Mechanism of nickel atoms with carbon dioxide  
J. Phys. Chem. A, 2000, 104, 11622-11627.
  115. Kaiser R.I., Mebel A.M., Lee Y.T.  
Crossed-beam reaction of electronically excited carbon atoms with  
hydrocarbon molecules I: Chemical dynamics of cyclopropynylethyne (c-C<sub>3</sub>H;  
X<sup>2</sup>B<sub>2</sub>) formation from reaction of C(<sup>1</sup>D) with acetylene, C<sub>2</sub>H<sub>2</sub>(X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>)  
J. Chem. Phys., 2001, 114, 231-239.
  116. Zyubin A.S., Mebel A.M., Chao S.D., Skodje R.T.  
Reaction dynamics of S(<sup>1</sup>D) + H<sub>2</sub>/D<sub>2</sub> on a new ab initio potential surface  
J. Chem. Phys., 2001, 114, 320-330.
  117. Yeh Y.L., Zhang C., Held H., Mebel A.M., Wei X., Lin S.H., Shen Y.R.  
Structure of the acetone liquid/vapor interface  
J. Chem. Phys., 2001, 114, 1837-1843.
  118. Charkin O.P., Klimenko N.M., Moran D., Mebel A.M., Schleyer P.v.R.  
Ab initio calculations of X@A<sub>12</sub>H<sub>12</sub><sup>2-</sup> closo alane and gallane anions with X  
atoms of inert gases or halogens inside the icosahedral [Al<sub>12</sub>] and [Ga<sub>12</sub>]  
clusters  
Russ. J. Inorg. Chem., 2001, 46, 110-120.
  119. Nguyen T.L., Le T.N., Mebel A.M.  
Thermochemistry of Cyclopentadienylidene (c-C<sub>5</sub>H<sub>4</sub>, C<sub>2v</sub>, <sup>3</sup>B<sub>1</sub>),  
Cyclopentadienyl Radical (c-C<sub>5</sub>H<sub>5</sub><sup>•</sup>, C<sub>2v</sub>, <sup>2</sup>B<sub>1</sub>), and 1,3-Cyclopentadiene (c-  
C<sub>5</sub>H<sub>6</sub>, C<sub>2v</sub>, <sup>1</sup>A<sub>1</sub>): A Theoretical Study by the G2M(RCC,MP2) Method  
J. Phys. Org. Chem., 2001, 14, 131-138.
  120. Mebel A.M., Baer M., Lin S.H.  
Ab initio study of nonadiabatic coupling matrix elements between excited 2<sup>2</sup>A'  
and 3<sup>2</sup>A' electronic states of C<sub>2</sub>H  
Chem. Phys. Lett., 2001, 336, 135-142.
  121. Kaiser R.I., Lee H.Y., Mebel A.M., Lee Y.T.  
Neutral-neutral reactions in the interstellar medium IV: The formation of C<sub>5</sub>H<sub>5</sub>  
isomers as potential key intermediates to PAH like molecules  
Astrophysical Journal, 2001, 548, 852-860.
  122. Le T.N., Lee H.Y., Mebel A.M., Kaiser R.I.  
  
Ab initio MO study of the triplet C<sub>3</sub>H<sub>4</sub> potential energy surface and the reaction  
of C(<sup>3</sup>P<sub>j</sub>) with ethylene, C<sub>2</sub>H<sub>4</sub>

- J. Phys. Chem. A, 2001, 105, 1847-1856.
123. Nguyen T.L., Mebel A.M., Kaiser R.I.  
A theoretical investigation of the triplet carbon atom  $C(^3P)$  + vinyl radical  $C_2H_3(^2A')$  reaction and thermochemistry of  $C_3H_n$  ( $n = 1-4$ ) species  
J. Phys. Chem. A, 2001, 105, 3284-3299.
124. Mebel A.M., Baer M., Lin S.H.  
Degenerate conical intersections: The interaction between the  $3^2A'$  and  $4^2A'$  electronic states of  $C_2H$  as a case study  
J. Chem. Phys., 2001, 114, 5109-5112.
125. Mebel A.M., Lin M.C., Chakraborty D., Park J., Lin S.H., Lee Y.T.  
Ab initio MO/RRKM study of multichannel rate constants for the  $H + C_6H_5$  reaction and the unimolecular decomposition of benzene  
J. Chem. Phys., 2001, 114, 8421-8435.
126. Mebel A.M., Hayashi M., Jackson W.M., Wrobel J., Green M., Xu D.D., Lin S.H.  
Branching ratios of  $C_2$  products in the photodissociation of  $C_2H$  at 193 nm  
J. Chem. Phys., 2001, 114, 9821-9831.
127. Nguyen T.L., Mebel A.M., Lin S.H.  
The role of the ground and excited potential energy surfaces in the  $O(^1D$  and  $^3P) + SiH_4$  reactions: A theoretical study  
J. Chem. Phys., 2001, 114, 10816-10834.
128. Hwang D.-Y., Mebel A.M.  
Theoretical study of the reaction mechanism of ScO with molecular hydrogen  
Chem. Phys. Lett., 2001, 341, 393-399.
129. Shu J., Lin J.J., Wang C.C., Lee Y.T., Yang X., Nguyen T.L., Mebel A.M.  
 $O(^1D)$  reaction with cyclopropane: Evidence of O atom insertion into the C-C bond  
J. Chem. Phys., 2001, 115, 7-10.
130. Le T.N., Mebel A.M., Kaiser R.I.  
An ab initio study of the  $C_4H_3$  potential energy surface and the reaction of  $C(^3P_j)$  with propargyl radical,  $HCCCH_2(X^2B_1)$   
J. Comput. Chem., 2001, 22, 1522-1535.
131. Mebel A.M., Hwang D.-Y.  
Theoretical study of the reaction mechanism of Fe atoms with  $H_2O$ ,  $H_2S$ ,  $O_2$ , and  $H^+$   
J. Phys. Chem. A, 2001, 105, 7460-7467.
132. Mebel A.M., Yahalom A., Englman R., Baer M.

The study of conical intersections between consecutive pairs of the five lowest  $^2A'$ -states of the  $C_2H$  molecule

- J. Chem. Phys., 2001, 115, 3673-3689.
133. Shiu Y.J., Hayashi M., Mebel A.M., Chen Y.-T., Lin S.H.  
Computational Formulas for Symmetry-forbidden Vibronic Spectra and Application to  $n\text{-}\pi^*$  Transition in Neat Acetone  
J. Chem. Phys., 2001, 115, 4080-4094.
  134. Balucani N., Lee H.-Y., Mebel A.M., Lee Y.T., Kaiser R.I.  
A combined crossed beam and ab initio investigation on the reaction of carbon species with  $\text{C}_4\text{H}_6$  isomers III: 1,2-butadiene,  $\text{H}_2\text{CCCH}(\text{CH}_3)$  ( $X^1A'$ ) – a non-RRKM system?  
J. Chem. Phys., 2001, 115, 5107-5116.
  135. Kaiser R.I., Mebel A.M., Lee Y.T., Chang A.H.H.  
Unimolecular decomposition of chemically activated triplet  $\text{C}_4\text{HD}_3$  complexes – a combined crossed beam and ab initio study  
J. Chem. Phys., 2001, 115, 5117-5125.
  136. Glinka Yu.D., Zyubin A.S., Mebel A.M., Lin S.H., Hwang L.P., Chen Y.T.  
Photoluminescence properties of silica-based mesoporous materials similar to those of nanoscale silicon  
Eur. Phys. J. D, 2001, 16, 279-283.
  137. Balucani N., Mebel A.M., Lee Y.T., Kaiser R.I.  
A combined crossed molecular beam and ab initio study of the reactions  $\text{C}_2(X^1\Sigma_g^+, a^3\Pi_u) + \text{C}_2\text{H}_4 \rightarrow n\text{-C}_4\text{H}_3(X^2A') + \text{H}(^2S_{1/2})$   
J. Phys. Chem. A, 2001, 105, 9813-9818.
  138. Baer M., Mebel A.M.  
Quantization of the Ab Initio Non-Adiabatic Coupling Matrix: The  $\text{C}_2\text{H}$  Molecule as a Case Study  
Int. J. Quantum Chem., 2001, 85, 315-326.
  139. Rozenbaum V.M., Mebel A.M., Lin S.H.  
Intermolecular potential and equilibrium orientational states for dimers of nonpolar molecule  
Mol. Phys., 2001, 99, 1883-1897.
  140. Hwang D.-Y., Mebel A. M.  
Theoretical study of the reaction of beryllium oxide with methane  
Chem. Phys. Lett., 2001, 348, 303-310.
  141. Hwang D.-Y., Mebel A.M.  
Conversion of CO to formaldehyde catalyzed by BeO: A theoretical study  
J. Phys. Chem. A, 2001, 105, 10433-10438.
  142. Kaiser R.I., Le T.N., Nguyen T.L, Mebel A.M., Balucani N., Lee Y.T., Stahl F., Schleyer P.v.R., Schaefer, III H.F.

- A combined crossed molecular beam and ab initio investigation of C<sub>2</sub> and C<sub>3</sub> elementary reactions with unsaturated hydrocarbons – pathways to hydrogen deficient radicals in combustion flames  
Faraday Discuss., 2001, 119, 51-66.
143. Xia W.S., Zhu R.S., Lin M.C., Mebel A.M.  
Low-Energy Paths for the Unimolecular Decomposition of CH<sub>3</sub>OH:  
A G2M/Statistical Theory Study  
Faraday Discuss., 2001, 119, 191-206.
144. Kaiser R.I., Nguyen T.L., Le T.N., Mebel A.M.  
An ab initio investigation of reactions of carbon atoms, C(<sup>3</sup>P<sub>j</sub>), with C<sub>2</sub>H<sub>4</sub> and C<sub>3</sub>H<sub>6</sub> in the interstellar media  
Astrophysical Journal, 2001, 561, 858-863.
145. Nguyen T.L., Kim G.-S., Mebel A.M., Nguyen M.T.  
A theoretical re-evaluation of the heat of formation of phenylcarbene  
Chem. Phys. Lett., 2001, 349, 571-577.
146. Zhu R.S., Diau E.W.G., Lin M.C., Mebel A.M.  
A computational study of the OH(OD) + CO reactions: Effects of pressure, temperature, and quantum-mechanical tunneling on product formation  
J. Phys. Chem. A, 2001, 105, 11249-11259.
147. Nguyen T.L., Mebel A.M., Lin S.H., Kaiser R.I.  
Product branching ratios of the C(<sup>3</sup>P) + C<sub>2</sub>H<sub>3</sub>(<sup>2</sup>A') and CH(<sup>2</sup>Π) + C<sub>2</sub>H<sub>2</sub>(<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) reactions and photodissociation of H<sub>2</sub>CC≡CH(<sup>2</sup>B<sub>1</sub>) at 193 and 242 nm: An ab initio RRKM study  
J. Phys. Chem. A, 2001, 105, 11549-11559.
148. Charkin O.P., Klimenko N.M., Moran D., Mebel A.M., Charkin D.O., Schleyer P.v.R.  
A Theoretical Study of Icosahedral Closo-Borane, Alane, and Gallane Dianions (A<sub>12</sub>H<sub>12</sub><sup>2-</sup>; A = B, Al, Ga) with Endohedral Noble Gas Atoms (Ng = He, Ne, Ar and Kr) and their Lithium Salts (Li[Ng@A<sub>12</sub>H<sub>12</sub>]<sup>-</sup> and Li<sub>2</sub>[Ng@A<sub>12</sub>H<sub>12</sub>])  
Inorg. Chem., 2001, 40, 6913-6922.
149. Lin S.H., Mishima K., Hayashi M., Chang A.H.H., Yi J., Mebel A.M.  
A theory of coulomb explosion of molecules  
J. Chin. Chem. Soc., 2001, 48, 963-969.
150. Mebel A.M., Kaiser R.I.  
The formation of interstellar C<sub>2</sub>N isomers in circumstellar envelopes of carbon stars: An ab initio study  
Astrophysical Journal, 2002, 564, 787-791.
151. Zyubin A.S., Glinka Yu.D., Mebel A.M., Lin S.H., Hwang L.P., Chen Y.T.

Red and Near-Infrared Photoluminescence from Silica-Based Nanoscale Materials: Experimental Investigation and Quantum Chemical Modeling

- J. Chem. Phys., 2002, 116, 281-294.
152. Kaiser R.I., Nguyen T.L., Mebel A.M., Lee Y.T.  
Stripping dynamics in the reactions of electronically excited carbon atoms,  $C(^1D)$ , with ethylene and propylene – production of propargyl and methylpropargyl radicals  
J. Chem. Phys., 2002, 116, 1318-1324.
153. Hwang D.-Y., Mebel A.M.  
Ab initio study of the reaction mechanisms of NiO and NiS with  $H_2$   
J. Phys. Chem. A, 2002, 106, 520-528.
154. Ho T.-S., Hollebeek T., Rabitz H., Chao S.D., Skodje R.T., Zyubin A.S., Mebel A.M.  
A globally smooth ab initio potential surface of the  $1A'$  state for the reaction  $S(^1D) + H_2$   
J. Chem. Phys., 2002, 116, 4124-4134.
155. Hwang D.-Y., Mebel A.M.  
An initio study of the reaction mechanism of  $CO_2$  with Ti atom in the ground and excited electronic states  
J. Chem. Phys., 2002, 116, 5633-5642.
156. Baer M., Mebel A.M., Englman R.  
Conical Intersection Revisited: Extension to an Elliptic Form  
Chem. Phys. Lett., 2002, 354, 243-250.
157. Wang C.C., Shu J., Lin J.J., Lee Y.T., Yang X., Nguyen T.L., Mebel A.M.  
Experimental and theoretical investigations of the  $O(^1D)$  reaction with cyclopropane  
J. Chem. Phys., 2002, 116, 8292-8299.
158. Hwang D.-Y., Mebel A.M.  
An initio study of the reaction mechanism of Sc atoms with carbon dioxide  
Chem. Phys. Lett., 2002, 357, 51-58.
159. Halasz G.J., Vibok A., Mebel A.M., Baer M.  
Ab initio nonadiabatic coupling elements: The conical intersection between the  $2^2A'$  and  $3^2A'$  of the  $H + H_2$  system  
Chem. Phys. Lett., 2002, 358, 163-169.
160. Glinka Yu.D., Zyubin A.S., Mebel A.M., Lin S.H., Hwang L.P., Chen Y.T.  
Photoluminescence from mesoporous silica akin to that from nanoscale silicon: The nature of light-emitters  
Chem. Phys. Lett., 2002, 358, 180-186.
161. Zyubin A.S., Mebel A.M., Lin S.H., Glinka Yu.D.  
Photoluminescence of Silanone and Dioxasilyrane Groups in Silicon Oxides: A Theoretical Study  
J. Chem. Phys., 2002, 116, 9889-9896.
162. Zyubina T.S., Kim G.-S., Lin S.H., Mebel A.M., Bandrauk A.D.

- Dissociation pathways of benzene trication  
Chem. Phys. Lett., 2002, 359, 253-261.
163. Mebel A.M., Kaiser R.I.  
An Ab Initio Study on the Formation of Interstellar Tricarbon Isomers I-  
C<sub>3</sub>(X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) and c-C<sub>3</sub>(X<sup>3</sup>A<sub>2</sub>' )  
Chem. Phys. Lett., 2002, 360, 139-143.
164. Kislov V.V., Mebel A.M., Lin S.H.  
Ab initio and DFT study of the formation mechanism of polycyclic aromatic  
hydrocarbons: The phenanthrene synthesis from biphenyl and naphthalene  
J. Phys. Chem. A, 2002, 106, 6171-6182.
165. Mebel A.M., Halasz G.J., Vibok A., Alijah A., Baer M.  
Quantization of the 3x3 non-adiabatic coupling matrix for three coupled states  
of the C<sub>2</sub>H molecule  
J. Chem. Phys., 2002, 117, 991-1000.
166. Baer M., Mebel A.M., Billing G.D.  
The necessary conditions for a rigorous minimal diabatic potential matrix  
J. Phys. Chem. A, 2002, 106, 6499-6507.
167. Kim G.-S., Mebel A.M., Lin S.H.  
Ab Initio Study of Excited Electronic States and Vibronic Spectra of Phenyl  
Radical  
Chem. Phys. Lett., 2002, 361, 421-431.
168. Lee H.Y., Mebel A.M., Lin S.H.  
An ab initio/RRKM study of photodissociation of carbonyl cyanide  
Int. J. Quantum Chem., 2002, 90, 566-574.
169. Schranz H.W., Smith S.C., Mebel A.M., Lin S.H., Lee Y.T.  
Prediction of absolute rate coefficients and product branching ratios for the  
C(<sup>3</sup>P) + allene reaction system  
J. Chem. Phys., 2002, 117, 7055-7067.
170. Hwang D.-Y., Mebel A.M.  
Theoretical study of the reaction mechanism of platinum oxide with methane  
Chem. Phys. Lett., 2002, 365, 140-147.
171. Charkin O.P., Charkin D.O., Klimenko N.M., Mebel A.M.  
A Theoretical Study of Isomerism in Doped Aluminum XAl<sub>12</sub> Clusters (X = B,  
Al, Ga, C, Si, Ge) with 40 Valence Electrons  
Chem. Phys. Lett., 2002, 365, 494-504.
172. Baer M., Mebel A.M., Billing G.D.  
The Curl Equations as Substratum for the Deviation of the Electronic Non-  
Adiabatic Coupling Terms  
Int. J. Quantum Chem., 2002, 90, 1577-1585.

173. Charkin O.P., Klimenko N.M., Moran D., Mebel A.M., Charkin D.O., Schleyer P.v.R.  
Theoretical Study of Salts of *Closo* Borane, Alane, and Gallane Anions with Cations of Light Metals Inside and Outside of Icosahedral Clusters [A<sub>12</sub>H<sub>12</sub><sup>2-</sup>] (A = B, Al, Ga)  
J. Phys. Chem. A, 2002, 106, 11594-11602.
174. Hwang D.-Y., Mebel A.M.  
Activation of Methane by Neutral Transition Metal Oxides (ScO, NiO, and PdO): A Theoretical Study  
J. Phys. Chem. A, 2002, 106, 12072-12083.
175. Kaiser R.I., Mebel A.M.  
The reactivity of ground state carbon atoms with unsaturated hydrocarbons in combustion flames and in the interstellar medium  
Int. Rev. Phys. Chem., 2002, 21, 307-356.
176. Hu S., Halasz G., Vibok A., Mebel A.M., Baer M.  
The curl-divergence equations for the electronic non-adiabatic coupling terms: Study of the C<sub>2</sub>H molecule and the H<sub>2</sub> + H system  
Chem. Phys. Lett., 2003, 367, 177-185.
177. Lee H.Y., Kislov V.V., Lin S.H., Mebel A.M., Neumark D.M.  
An ab initio/RRKM study of product branching ratios in photodissociation of 1,2- and 1,3-butadienes and 2-butyne at 193 nm  
Chem. Eur. J., 2003, 9, 726-740.
178. Halasz G., Vibok A., Mebel A.M., Baer M.  
A survey of ab initio conical intersections for the H + H<sub>2</sub> system  
J. Chem. Phys., 2003, 118, 3052-3064.
179. Englman R., Yahalom A., Baer M., Mebel A.M.  
Multiple conical intersections: Observational aspects of topological phases  
Int. J. Quantum Chem., 2003, 92, 135-151.
180. Zyubin A.S., Mebel A.M.  
Performance of time-dependent density functional and Green functions methods for calculations of excitation energies in radicals and for Rydberg electronic states  
J. Comput. Chem., 2003, 24, 692-700.
181. Kim G.-S., Nguyen T.L., Mebel A.M., Lin S.H., Nguyen M.T.  
An ab initio/RRKM study of the potential energy surface of triplet ethylene and product branching ratios of the C(<sup>3</sup>P) + CH<sub>4</sub> reaction  
J. Phys. Chem. A, 2003, 107, 1788-1796.
182. Billing G.D., Baer M., Mebel A.M.  
Absorption cross section of C<sub>2</sub>H: Effect of proper treatment of the conical intersection  
Chem. Phys. Lett., 2003, 372, 1-7.
183. Hwang D.-Y., Mebel A.M.

- Reaction mechanism of N<sub>2</sub>/H<sub>2</sub> conversion to NH<sub>3</sub>: A theoretical study  
J. Phys. Chem. A, 2003, 107, 2865-2874.
184. Nguyen T.L., Mebel A.M., Kaiser R.I.  
Potential energy surface and product branching ratios for the reaction of C(<sup>3</sup>P<sub>j</sub>) with the allyl radical: An ab initio/RRKM study.  
J. Phys. Chem. A, 2003, 107, 2990-2999.
185. Zyubina T.S., Shilov G.V., Dobrovol'skii Y.A., Leonova L.S., Mebel A.M.  
Modeling the proton transport in orthoperiodic and orthotelluric acids and their salts  
Russ. J. Electrochem. 2003, 39, 376-385.
186. Hwang D.-Y., Mebel A.M.  
Reaction mechanism of the synthesis of ammonia in the N<sub>2</sub>/H<sub>2</sub>/BeO and N<sub>2</sub>/H<sub>2</sub>/FeO system: A theoretical study  
J. Phys. Chem. A, 2003, 107, 5092-5100.
187. Hwang D.-Y., Mebel A.M.  
Reaction mechanism of nitrogen hydrogenation in the presence of scandium oxide: A density functional study  
Chem. Phys. Lett., 2003, 375, 17-25.
188. Chin C.-H., Mebel A.M., Hwang D.-Y.  
Theoretical study of the reaction mechanism of boron atom with carbon dioxide  
Chem. Phys. Lett., 2003, 375, 670-675.
189. Zyubina T.S., Kim G.-S., Mebel A.M., Lin S.H., Bandrauk A.D.  
Ab initio/RRKM study of dissociation mechanism of benzene trication  
J. Theor. Comput. Chem., 2003, 2, 205-231.
190. Nguyen M.T., Nguyen T.L., Mebel A.M., Flammang R.  
Azido-Nitrene is probably the N<sub>4</sub> molecule observed in mass spectrometric experiments  
J. Phys. Chem. A, 2003, 107, 5452-5460.
191. Huang, C.-L., Jiang, J.-C., Mebel, A. M., Lee, Y. T., Ni, C.-K.  
Photodissociation Dynamics of Fluorobenzene  
J. Am. Chem. Soc., 2003, 125, 9814-9820.
192. Charkin O.P., Charkin D.O., Klimenko N.M., Mebel A.M.  
A theoretical study of isomerism in doped aluminum MAI<sub>12</sub> and MAI<sub>12</sub>X<sub>12</sub> clusters with 40 and 50 valence electrons  
Faraday Discuss., 2003, 124, 215-237.
193. Zyubina T.S., Shilov G.V., Dobrovol'skii Y.A., Leonova L.S., Nikitina Z.K., Chernyak A.V., Romanchenko E.V., Mebel A.M.  
Quantum-chemical simulation of the proton transport in mono- and disubstituted salts with octahedral anions  
Russ. J. Electrochem. 2003, 39, 600-606.
194. Sun Y.-C., Wang I.T., Nguyen T.L., Lu H.-F., Yang X., Mebel A.M.

- A Combined Quantum Chemistry and RRKM Calculation Predicts the  $O(^1D) + C_2H_6$  Reaction Can Produce Water Molecule in Collision-free Crossed Molecular Beam Environment  
J. Phys. Chem. A, 2003, 107, 6986-6994.
195. Zyubin A.S., Mebel A.M.  
Accurate prediction of excitation energies to high-lying Rydberg electronic states: Rydberg states of acetylene as a case study  
J. Chem. Phys., 2003, 119, 6581-6587.
196. Lin M.-F., Huang C.-L., Kislov V.V., Mebel A.M., Lee Y.T., Ni C.-K.  
H and  $CH_3$  eliminations in the photodissociation of chlorotoluene  
J. Chem. Phys., 2003, 119, 7701-7704.
197. Liang K.K., Mebel A.M., Lin S.H., Hayashi M., Selzle H.L., Schlag E.W., Tachiya M.  
Influence of distortion and Duschinsky effects on Marcus-type theories of electron transfer rate  
Phys. Chem. Chem. Phys., 2003, 5, 4656-4665.
198. Zyubin A.S., Mebel A.M., Lin S.H.  
Quantum chemical modeling of photoabsorption and photoluminescence of the  $[AlO_4]^0$  defect in bulk  $SiO_2$   
J. Chem. Phys., 2003, 119, 11408-11414.
199. Kaiser R.I., Balucani N., Charkin D.O., Mebel A.M.  
A crossed beam and ab initio study of the  $C_2(X^1\Sigma_g^+/a^3\Pi_u) + C_2H_2(X^1\Sigma_g^+)$  reactions  
Chem. Phys. Lett., 2003, 382, 112-119.
200. Kislov V.V., Nguyen T.L., Mebel A.M., Lin S.H., Smith S.C.  
Photodissociation of benzene under collision-free conditions: An ab initio RRKM study  
J. Chem. Phys., 2004, 120, 7008-7017.
201. Chin C.-H., Mebel A.M., Hwang D.-Y.  
Theoretical study of the reaction mechanism of BO,  $B_2O_2$  and BS with  $H_2$   
J. Phys. Chem. A, 2004, 108, 473-483.
202. Bennett C.J., Jamieson C., Mebel A.M., Kaiser R.I.  
Untangling the formation of the cyclic carbon trioxide isomer in low temperature carbon dioxide ices  
Phys. Chem. Chem. Phys., 2004, 6, 735-746.
203. Charkin O.P., Klimenko N.M., Charkin D.O., Mebel A.M.  
Theoretical study of host-guest interaction in model endohedral fullerenes with  $CH_4$  and  $He_4$  into the  $C_{60}H_{36}$ ,  $C_{60}H_{24}$ ,  $C_{84}$ , and  $C_{60}$  cages  
Russ. J. Inorg. Chem., 2004, 49, 723-733.
204. Trakhtenberg L.I., Fokeyev A.A., Dolin S.P., Mebel A.M., Lin S.H.

- Rate Constant for H-Atom Tunneling in the Fluorene-Acridine System Based on DFT Potential Energy Surface  
Chem. Phys., 2004, 303, 107-113.
205. Charkin O.P., Klimenko N.M., Charkin D.O., Mebel A.M.  
Theoretical study of host-guest interaction in model endohedral fullerenes with tetrahedral molecules and ions of MH<sub>4</sub> hydrides inside the C<sub>60</sub>H<sub>36</sub>, C<sub>60</sub>H<sub>24</sub>, C<sub>84</sub>, and C<sub>60</sub> cages  
Russ. J. Inorg. Chem., 2004, 49, 868-880.
  206. Zyubina T.S., Shilov G.V., Dobrovolsky Yu.A., Leonova L.S., Mebel A.M.  
Singularity of proton transport in salts of ortho-periodic acids: Theoretical modeling using density functional calculations  
Dalton Trans., 2004, 2170-2179.
  207. Zyubina T.S., Lin S.H., Bandrauk A.D., Mebel A.M.  
Dissociation pathways of cyclohexane trication  
Chem. Phys. Lett., 2004, 393, 470-477.
  208. Tseng C.-M., Dyakov Y.A., Huang C.-L., Mebel A.M., Lin S.H., Lee Y.T., Ni C.-K.  
Photoisomerization and photodissociation of aniline and 4-methylpyridine  
J. Am. Chem. Soc., 2004, 126, 8760-8768.
  209. Vibok A., Halasz G., Mebel A.M., Hu S., Baer M.  
An analytic-numeric approach to calculate electronic non-adiabatic coupling terms: Study of the C<sub>2</sub>H molecule and the H<sub>2</sub>+H system  
Int. J. Quantum Chem., 2004, 99, 594-604.
  210. Hwang D.-Y., Mebel A.M.  
Reaction mechanism of hydrogenation of carbon dioxide to formic acid in the presence of scandium oxide: A density functional study  
Chem. Phys. Lett., 2004, 396, 75-82.
  211. Hwang D.-Y., Mebel A.M.  
Theoretical study of the reaction mechanism of nitrogen hydrogenation on transition metal oxides (TiO, VO, and CuO)  
Chem. Phys., 2004, 304, 301-313.
  212. Mebel A.M., Hayashi M., Kislov V.V., Lin S.H.  
Theoretical study of oxygen isotope exchange and quenching in the O(<sup>1</sup>D) + CO<sub>2</sub> reaction  
J. Phys. Chem. A, 2004, 108, 7983-7994.
  213. Charkin O.P., Klimenko N.M., Charkin D.O., Mebel A.M.  
Theoretical Study of Isomerism in Doped Aluminides LAI<sub>12</sub>  
Russ. J. Inorg. Chem., 2004, 49, 1382-1391.
  214. Charkin O.P., Klimenko N.M., Charkin D.O., Mebel A.M.

- Ab Initio Study of Host–Guest Interaction in Model Endohedral Fullerenes with Noble Gas Clusters Ng<sub>4</sub> (Ng = He, Ne, Ar, Kr, Xe) inside the C<sub>60</sub>H<sub>36</sub> and C<sub>84</sub> Cages  
 Russ. J. Inorg. Chem., 2004, 49, 1392-1402.
215. Charkin O.P., Klimenko N.M., Charkin D.O., Mebel A.M., Schleyer P.v.R.  
 Theoretical Study of Isomerism in Alanes LAI<sub>12</sub>H<sub>12</sub> with Metal Cations Inside and Outside of the Icosahedral Anion Al<sub>12</sub>H<sub>12</sub><sup>2-</sup>  
 Russ. J. Inorg. Chem., 2004, 49, 1536-1546.
216. Hwang D.-Y., Mebel A.M.  
 Theoretical study of TiO-catalyzed hydrogenation of carbon dioxide to formic acid  
 J. Phys. Chem. A, 2004, 108, 10245-10251.
217. Wang L., Mebel A.M., Yang X., Wang X.  
 Ab initio/RRKM study of the O(<sup>1</sup>D) + NH<sub>3</sub> reaction: Product branching ratios  
 J. Phys. Chem. A, 2004, 108, 11644-11650.
218. Charkin O.P., Klimenko N.M., Charkin D.O., Mebel A.M.  
 Theoretical study of the association of icosahedral doped aluminide clusters: (L@Al<sub>12</sub>)<sub>2</sub> and (L@Al<sub>12</sub>)(L'@Al<sub>12</sub>) dimers (L, L' = Si and Ge)  
 Russ. J. Inorg. Chem., 2004, 49, 1898-1905.
219. Hayes M., Gustafsson M., Mebel A.M., Skodje R.T.  
 An Improved Potential Energy Surface for the F+H<sub>2</sub> Reaction  
 Chem. Phys., 2005, 308, 259-266.
220. Shieh J.-C., Wu J.-C., Li R., Chang J.-I., Lin Y.-J., Liao D.-W., Hayashi M., Mebel A.M., Handy N.C., Chen Y.-T.  
 Two-photon vibronic spectroscopy of Rydberg states of allene at 7.0-10.5 eV: Experiment and theory  
 Mol. Phys., 2005, 103, 229-248.
221. Charkin O.P., Klimenko N.M., Charkin D.O., Mebel A.M., Schleyer P.v.R.  
 Theoretical study of the isomerism of stepwise-hydrogenated aluminum clusters Al<sub>13</sub>H<sub>2n</sub><sup>-</sup> (n=0-6) with the centered icosahedral Al<sub>13</sub> framework  
 Russ. J. Inorg. Chem., 2005, 50, 50-60.
222. Mebel A.M., Zyubina T.S., Dyakov Y.A., Bandrauk A.D., Lin S.H.  
 Potential energy surfaces in Coulomb explosion of polyatomic molecules  
 Int. J. Quantum Chem., 2005, 102, 506-519.
223. Wang L., Kislov V.V., Mebel A.M., Yang X., Wang X.  
 Potential energy surface and product branching ratios for the reaction of F(<sup>2</sup>P) with the methyl radical: An ab initio/RRKM study  
 Chem. Phys. Lett., 2005, 406, 60-74.
224. Budyka M.F., Zyubina T.S., Ryabenko A.G., Lin S.H., Mebel A.M.

- Bond lengths and diameters of armchair single wall carbon nanotubes  
Chem. Phys. Lett., 2005, 407, 266-271.
225. Jamieson C.S., Bennett C.J., Mebel A.M., Kaiser R.I.  
Investigating the mechanism for the formation of nitrous oxide  $N_2O(X^1\Sigma^+)$  in  
extraterrestrial ices  
Astrophys. J., 2005, 624, 436-447.
226. Tokmakov I.V., Kim G.-S., Kislov V.V., Mebel A.M., Lin M.C.  
The reaction of phenyl radical with molecular oxygen: A G2M study of the  
potential energy surface  
J. Phys. Chem. A, 2005, 109, 6114-6127.
227. Charkin O.P., Klimenko N.M., Charkin D.O., Mebel A.M.  
Isomerism of doped aluminum clusters with the icosahedral  $Al_{12}$  cage  
Russ. J. Inorg. Chem., 2005, 50, Suppl. 1, S17-S40.
228. Zyubin A.S., Mebel A.M., Lin S.H.  
Photoluminescence of oxygen-containing surface defects in germanium  
oxides: A theoretical study  
J. Chem. Phys., 2005, 123, 044701 (14 pp.).
229. Lin M.-F., Dyakov Y.A., Tseng C.-M., Mebel A.M., Lin S.H., Lee, Y.T., Ni C.-K.  
Photodissociation dynamics of pyridine  
J. Chem. Phys., 2005, 123, 054309 (11 pp.).
230. Mebel A.M., Kislov V.V.  
The  $C_2H_3 + O_2$  Reaction Revisited: Is Multireference Treatment of the Wave  
Function Really Critical?  
J. Phys. Chem. A, 2005, 109, 6993-6997.
231. Kislov V.V., Islamova N.I., Kolker A.M., Lin S.H., Mebel A.M.  
Hydrogen abstraction acetylene addition and Diels-Alder mechanisms of PAH  
formation: A detailed study using first principles calculations  
J. Chem. Theor. Comp., 2005, 1, 908-924.
232. Trakhtenberg L. I., Fokeyev A.A., Dolin S.P., Mebel A.M., Lin S.H.  
Temperature and pressure dependence of tunneling rate constant. DFT  
potential energy surface for H-atom transfer in the fluorene-acredine system  
J. Chem. Phys., 2005, 123, 114508 (12 pp.).
233. Dyakov Y.A., Ni C.K., Lin S.H., Lee Y.T., Mebel A.M.  
Photodissociation of azulene at 193 nm: Ab initio and RRKM study  
J. Phys. Chem. A, 2005, 109, 8774 - 8784.
234. Zyubina T.S., Dyakov Y.A., Lin S.H., Bandrauk A.D., Mebel A.M.  
Theoretical study of isomerization and dissociation of acetylene dication in the  
ground and excited electronic states  
J. Chem. Phys., 2005, 123, 134320 (13 pp.).

235. Charkin O.P., Klimenko N.M., Nguyen P.T., Charkin D.O., Mebel A.M., Lin S.H., Wang Y.-S., Wei S.-C., Chang H.-C.  
Fragmentation of heme and hemin<sup>+</sup> with sequential loss of carboxymethyl groups: A DFT and mass-spectrometry study  
Chem. Phys. Lett., 2005, 415, 362-369.
236. Jamieson C.S., Mebel A.M., Kaiser R.I.  
A matrix isolation study of the C<sub>s</sub> symmetric OCNO(X<sup>2</sup>A') radical  
Phys. Chem. Chem. Phys., 2005, 7, 4089-4095.
237. Charkin O.P., Klimenko N.M., Charkin D.O., Mebel A.M.  
Ab Initio Study of Host–Guest Interaction in Model Endohedral Fullerenes with Benzene and Borazole Molecules inside the C<sub>84</sub> (D<sub>6h</sub>) Cage  
Russ. J. Inorg. Chem., 2005, 50, 1702-1709.
238. Charkin O.P., Klimenko N.M., Charkin D.O., Mebel A.M.  
Theoretical Study of Host–Guest Interaction in Model Endohedral Fullerenes with Linear Triatomic and Tetratomic Molecules inside the C<sub>70</sub> (D<sub>5h</sub>) Cage  
Russ. J. Inorg. Chem., 2005, 50, 1903-1911.
239. Zyubin A.S., Mebel A.M., Lin S.H.  
Quantum-Chemical Simulation of the Optical Properties of O=X and O<sub>2</sub>X< Point Defects in Silicon and Germanium Oxides  
Russ. J. Inorg. Chem., 2005, 50, 1912-1920.
240. Mebel A.M., Kislov V.V., Kaiser R.I.  
Potential energy surface and product branching ratios for the reaction of dicarbon, C<sub>2</sub>(X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>), with methylacetylene, CH<sub>3</sub>CCH(X<sup>1</sup>A<sub>1</sub>): An ab initio/RRKM study  
J. Phys. Chem. A, 2006, 110, 2421-2433 (Cover page article).
241. Wang P., Woo H.K., Lau K.-C., Xing X., Ng C.Y., Zyubin A.S., Mebel A.M.  
Infrared vibrational spectroscopy of *cis*-dichloroethene in Rydberg states  
J. Chem. Phys., 2006, 124, 064310 (7 pp).
242. Lin M.-F., Dyakov Y.A., Tseng C.-M., Mebel A.M., Lin S.H., Lee, Y.T., Ni C.-K.  
Photodissociation dynamics of pyrimidine  
J. Chem. Phys., 2006, 124, 084303 (8 pp.).
243. Dyakov Y.A., Mebel A.M., Lin S.H., Lee Y.T., Ni C.K.  
Acetylene elimination in photodissociation of neutral azulene and its cation: An ab initio and RRKM study  
J. Chin. Chem. Soc., 2006, 53, 161-168.
244. Dyakov Y.A., Ni C.K., Lin S.H., Lee Y.T., Mebel A.M.

- Ab initio and RRKM study of photodissociation of azulene cation  
 Phys. Chem. Chem. Phys., 2006, 12, 1404-1415.
245. Jamieson C.S., Mebel A.M., Kaiser R.I.  
 Understanding the kinetics and dynamics of radiation induced reaction pathways in carbon monoxide ice at 10 K  
 Astrophys. J., Suppl. Series, 2006, 206, 163-184.
246. Zyubin A.S., Mebel A.M., Lin S.H.  
 Photoluminescence of oxygen-deficient defects in germanium oxides: A quantum chemical study  
 J. Chem. Phys., 2006, 125, 064701 (9 pp.).
247. Cheng B.-M., Lu H.-C., Chen H.-K., Bahou M., Lee Y.-P., Mebel A.M., Lee L.C., Liang M.-C., Yung Y.L., Absorption cross sections of NH<sub>3</sub>, NH<sub>2</sub>D, NHD<sub>2</sub>, and ND<sub>3</sub> in the spectral range 140-220 nm and its implication to planetary isotopic fractionation, Astrophys. J., 2006, 647, 1535-1542.
248. Guo Y., Gu X., Zhang F., Mebel A.M., Kaiser R.I., Unimolecular decomposition of chemically activated pentatetraene (H<sub>2</sub>CCCCCH<sub>2</sub>) intermediates: A crossed beams study of dicarbon molecule reactions with allene, J. Phys. Chem. A, 2006, 110, 10699-10707.
249. Gu X., Guo Y., Mebel A.M., Kaiser R.I., Chemical dynamics of the formation of the 1,3-butadiynyl radical (C<sub>4</sub>H(X<sup>2</sup>Σ<sup>+</sup>)) and its isotopomers, J. Phys. Chem. A, 2006, 110, 11265-11278.
250. Mebel A.M., Kislov V.V., Kaiser R.I., Ab initio/RRKM study of the singlet C<sub>4</sub>H<sub>4</sub> potential energy surface and of the reactions of C<sub>2</sub>(X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) with C<sub>2</sub>H<sub>4</sub>(X<sup>1</sup>A<sub>1g</sub><sup>+</sup>) and C(<sup>1</sup>D) with C<sub>3</sub>H<sub>4</sub> (allene and methylacetylene), J. Chem. Phys., 2006, 125, 133113 (15 pp.).
251. Gu X., Guo Y., Zhang F., Mebel A.M., Kaiser R.I., Reaction dynamics of carbon bearing radicals in circumstellar envelopes of carbon stars, Faraday Discuss., 2006, 133, 245-275.
252. Jamieson C.S., Mebel A.M., Kaiser R.I., Identification of the D<sub>3h</sub> isomer of carbon trioxide (CO<sub>3</sub>) and its implications for atmospheric chemistry, ChemPhysChem, 2006, 7, 2508-2513.
253. Guo Y., Kislov V.V., Gu X., Zhang F., Mebel A.M., Kaiser R.I.  
 A combined experimental and theoretical study of the reaction of dicarbon (C<sub>2</sub>) with D<sub>1</sub> acetylene (HCCD): Possible mechanisms for deuterium enrichment in the interstellar D<sub>1</sub>-butadiynyl radical, CCCCD(X<sup>2</sup>Σ<sup>+</sup>)  
 Astrophys. J., 2006, 653, 1577-1582.
254. Zyubin A.S., Mebel A.M., Lin S.H.

- Quantum-chemical modeling of interaction of point defects  $O = X<$  and  $O_2X<$  in silicon and germanium oxides: photoabsorption and photoluminescence. *Izvestia of Russ. Acad. Sci., Ser. Fiz.* 2006, 70 1151-1159.
255. Charkin O.P., Klimenko N.M., Charkin D.O., Mebel A.M.  
Theoretical study of isomerism, structure, and stability of dimers of C-doped aluminum clusters  $(C@Al_{12})_2$  and  $(C@Al_{12})(L@Al_{12})$  ( $L = Si, Ge$ )  
*Russ. J. Inorg. Chem.* 2006, 51, 652-661.
256. Zyubina T.S., Razumov V.F., Brichkin S.B., Anisimov V., Lin S.H., Mebel A.M..  
Quantum-chemical study of crystal formation of supramolecular silver compounds with trans-1,2-bis(4-pyridyl)ethylene and their electronic absorption spectra.  
*Russ. J. Inorg. Chem.* 2006, 51, 996-1011.
257. Gu X., Guo Y., Zhang F., Mebel A.M., Kaiser R.I.  
A crossed molecular beam study of the reaction of dicarbon molecules with benzene – identification of the phenylethynyl radical ( $C_6H_5CC$ ;  $X^2A'$ )  
*Chem. Phys. Lett.*, 2007, 436, 7-14.
258. Guo Y., Gu X., Zhang F., Mebel A.M., Kaiser R.I.  
A crossed molecular beam study on the formation of hexenediynyl radical ( $H_2CCCCCCH$ ;  $C_6H_3$  ( $X^2A'$ )) via reactions of tricarbon molecules,  $C_3(X^1\Sigma_g^+)$  with allene ( $H_2CCCH_2$ ;  $X^1A_1$ ) and methylacetylene ( $CH_3CCH$ ;  $X^1A_1$ )  
*Phys. Chem. Chem. Phys.*, 2007, 16, 1972-1979. (Cover page article)
259. Kislov V.V., Mebel A.M.  
An ab initio G3-type / statistical theory study of the formation of indene in combustion flames. I. The pathways involving benzene and phenyl radical  
*J. Phys. Chem. A*, 2007, 111, 3922-3931.
260. Jamieson C.S., Mebel A.M., Kaiser R.I.  
Novel identification of the  $C_{2v}$  isomer of carbon tetraoxide ( $CO_4$ )  
*Chem. Phys. Lett.*, 2007, 440, 105-109.
261. Guo Y., Mebel A.M., Zhang F., Gu X., Kaiser R.I.  
Crossed molecular beam studies of the reactions of allyl radicals,  $C_3H_5(X^2A_1)$ , with methylacetylene ( $CH_3CCH(X^1A_1)$ ), allene ( $H_2CCCH_2(X^1A_1)$ ), and their isotopomers  
*J. Phys. Chem. A*, 2007, 111, 4914-4921.
262. Gu X., Guo Y., Zhang F., Mebel A.M., Kaiser R.I.  
A crossed molecular beam study on the formation and energetics of the resonantly stabilized free i- $C_4H_3(X^2A')$  radical and its isotopomers  
*Chem. Phys.*, 2007, 335, 95-108.
263. Mebel A.M., Kislov V.V., Hayashi M.

- Prediction of product branching ratios in the  $C(^3P) + C_2H_2 \rightarrow I-C_3H + H/c-C_3H + H/C_3 + H_2$  reaction using ab initio coupled clusters/complete basis set calculations combined with RRKM and radiationless transition theories  
*J. Chem. Phys.*, 2007, 126, 204310 (11 pp.).
264. Joshi S.S., Mebel A.M.  
 Computational modeling of biodegradable composites of the starch component amylose and poly(propylene carbonate)  
*Polymer*, 2007, 48, 3893-3901.
265. Mebel A.M., Kim G.-S., Kislov V.V., Kaiser R.I.  
 The reaction of tricarbon with acetylene: An ab initio/RRKM study of the potential energy surface and product branching ratios  
*J. Phys. Chem. A*, 2007, 111, 6704-6712.
266. Yao L., Mebel A.M., Lu H.F., Nausser H.J., Lin S.H.  
 Anharmonic effect on unimolecular reactions with application to the photodissociation of ethylene  
*J. Phys. Chem. A*, 2007, 111, 6722-6729.
267. Longenecker J.G., Mebel A.M., Kaiser R.I.  
 First infrared spectroscopic detection of the monobridged diboranyl radical ( $B_2H_5; C_{2v}$ ) and its D5 isotopomer in low temperature diborane ices  
*Inorg. Chem.*, 2007, 46, 5739-5743.
268. Jamieson C.S., Mebel A.M., Kaiser R.I.  
 First detection of the  $C_2$  Symmetric Isomer of carbon pentaoxide ( $CO_5$ ) at 10 K  
*Chem. Phys. Lett.*, 2007, 443, 49-54.
269. Xu T., Kamat P.V., Joshi S., Mebel A.M., Cai Y., O'Shea K.E.  
 Hydroxyl radical mediated degradation of phenylarsonic acid  
*J. Phys. Chem. A*, 2007, 111, 7819-7824.
270. Lin M.-F., Dyakov Y.A., Lee Y.T., Lin S.H., Mebel A.M., Ni C.-K.  
 Photodissociation of S atom containing amino acid chromophores  
*J. Chem. Phys.*, 2007, 127, 064308 (9 pages).
271. Gu X., Guo Y., Zhang F., Mebel A.M., Kaiser R.I.  
 Unimolecular Decomposition of Chemically Activated Singlet and Triplet D3-Methyldiacetylene Molecules  
*Chem. Phys. Lett.*, 2007, 444, 220-225.
272. Chin C.H., Mebel A.M., Kim G.S., Baek K.Y., Kim S.K., Hayashi M., Liang K.K., Lin S.H.  
 Theoretical investigations of spectroscopy and excited state dynamics of adenine  
*Chem. Phys. Lett.*, 2007, 445, 361-369.

273. Sharifi M., Kong F., Chin S.L., Mineo H., Dyakov Y., Mebel A.M., Chao S.D., Hayashi M., Lin S.H.  
Experimental and Theoretical Investigation of High-power Laser Ionization and Dissociation of Methane  
J. Phys. Chem. A, 2007, 111, 9405-9416.
274. Zyubin A.S., Mebel A.M., Lin S.H.  
Optical properties of oxygen vacancies in germanium oxides: quantum chemical modeling of photo-excitation and photo-luminescence  
J. Phys. Chem. A, 2007, 111, 9479-9485.
275. Kislov V.V., Mebel A.M.  
The formation of naphthalene, azulene, and fulvalene from the recombination product of two cyclopentadienyl radicals: An ab initio/RRKM study of rearrangements of the C<sub>5</sub>H<sub>5</sub>-C<sub>5</sub>H<sub>4</sub> (9-H-fulvalenyl) radical  
J. Phys. Chem. A, 2007, 111, 9532-9543.
276. Dyakov Y.A., Mebel A.M., Lin S.H., Lee Y.T. Ni C.-K.  
Photodissociation of 1,3,5-Triazine: An Ab Initio and RRKM Study  
J. Phys. Chem. A, 2007, 111, 9591-9599.
277. Gu X., Guo Y., Mebel A.M., Kaiser R.I.  
A crossed beam investigation of the reactions of tricarbon molecules, C<sub>3</sub>(X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>), with acetylene, C<sub>2</sub>H<sub>2</sub>(X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>), ethylene, C<sub>2</sub>H<sub>4</sub>(X<sup>1</sup>A<sub>g</sub>), and benzene, C<sub>6</sub>H<sub>6</sub>(X<sup>1</sup>A<sub>1g</sub>)  
Chem. Phys. Lett., 2007, 449, 44-52.
278. Zyubin A.S., Dembovskii S.A., Mebel A.M.  
Electronic excitations of hypervalent configurations in amorphous selenium: Quantum-chemical modeling  
Russ. J. Inorg. Chem., 2007, 52, 1407-1414.
279. Jamieson C.S., Mebel A.M., Kaiser R.I.  
First detection of the C<sub>s</sub> symmetric isomer of carbon hexaoxide (CO<sub>6</sub>) at 10 K  
Chem. Phys. Lett., 2008, 450, 312-317.
280. Kislov V.V., Mebel A.M.  
An Ab Initio G3-type / Statistical Theory Study of the Formation of Indene in Combustion Flames. II. The Pathways Originated from Reactions of Cyclic C<sub>5</sub> a Species - Cyclopentadiene and Cyclopentadienyl Radical  
J. Phys. Chem. A, 2008, 112, 700-716.
281. Gu X., Kaiser R.I., Mebel A.M.  
Chemistry of energetically activated cumulenes – from allene (H<sub>2</sub>CCCH<sub>2</sub>) to hexapentaene (H<sub>2</sub>CCCCCCH<sub>2</sub>)  
ChemPhysChem, 2008, 9, 350-369.
282. Zyubina T.S., Mebel A.M., Hayashi M., Lin S.H.

Theoretical study of multiphoton ionization of cyclohexadienes and unimolecular decomposition of their mono- and dications

- Phys. Chem. Chem. Phys., 2008, 10, 2321 - 2331.
283. Theoretical study of the C<sub>6</sub>H<sub>3</sub> potential energy surface and rate constants and product branching ratios of the C<sub>2</sub>H(<sup>2</sup>Σ<sup>+</sup>) + C<sub>4</sub>H<sub>2</sub> (<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) and C<sub>4</sub>H(<sup>2</sup>Σ<sup>+</sup>) + C<sub>2</sub>H<sub>2</sub> (<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) reactions  
Landera A., Krishtal S.P., Kislov V.V., Mebel A.M., Kaiser R.I.  
J. Chem. Phys., 2008, 128, 214301.
284. Theoretical study of the reaction mechanism of ethynyl radical with benzene and related reactions on the C<sub>8</sub>H<sub>7</sub> potential energy surface  
Landera A., Mebel A.M., Kaiser R.I.  
Chem. Phys. Lett., 2008, 459, 54-59.
285. Silva R., Gichuhi W.K., Huang C., Doyle M.B., Kislov V.V., Mebel A.M. Suits A. G.  
H elimination and metastable lifetimes in the UV photoexcitation of diacetylene  
Proc. Nat. Acad. Sci., 2008, 105, 12713-12718.
286. Zyubin A.S., Mebel A.M., Chang H.C., Lin S.H.  
Potential Energy Surfaces for the Lowest Excited States of the Nitrogen-Vacancy Point Defects in Diamonds: A Quantum Chemical Study  
Chem. Phys. Lett., 2008, 462, 251-255.
287. Kaiser R.I., Mebel A.M.  
On the formation of higher carbon oxides in extreme environments  
Chem. Phys. Lett., 2008, 465, 1-9. (Frontiers Article)
288. Mebel A.M., Kislov V.V., Kaiser R.I.  
On a Photo-Induced Mechanism of the Formation and Growth of Polycyclic Aromatic Hydrocarbons in Low-Temperature Environments via Successive Ethynyl Radical Additions  
J. Am. Chem. Soc., 2008, 130, 13618-13629.
289. Wang Q., Wu D., Jin M., Liu F., Hu F., Cheng X., Liu H., Hu Z., Ding D., Mineo H., Dyakov Y.A., Mebel A.M., Chao S.D., Lin S.H.  
Experimental and theoretical investigation of ionization / dissociation of cyclopentanone molecule in a femtosecond laser field  
J. Chem. Phys., 2008, 129, 204302 (15 pp.).
290. Mebel A.M., Bandrauk A.D.  
Theoretical study of unimolecular decomposition of allene cations  
J. Chem. Phys., 2008, 129, 224311 (12 pp.).
291. Zyubin A.S., Mebel A.M., Hayashi M., Chang H.C., Lin S.H.  
Quantum chemical modeling of photo-adsorption properties of the nitrogen-vacancy point defect in diamond  
J. Comput. Chem., 2009, 30, 119-131.
292. Zhang F., Kim S., Kaiser R.I., Mebel A.M.

- On the Formation of the 1,3,5-Hexatriynyl Radical ( $C_6H(X^2\Sigma^+)$ ) via the Crossed Beams Reaction of Dicarbon ( $C_2(X^1\Sigma_g^+/a^3\Pi_u)$ ), with Diacetylene ( $C_4H_2(X^1\Sigma_g^+)$ )  
 J. Phys. Chem. A, 2009, 113, 1210-1217.
293. Yao L., He R.X., Mebel A.M., Lin S.H.  
 On the calculation of the dissociation rate constant of the water dimer by the ab initio anharmonic RRKM theory  
 Chem. Phys. Lett., 2009, 470, 210-214.
294. Trakhtenberg L.I., Fokeyev A.A., Zyubin A.S., Mebel A.M., Lin S.H.  
 Matrix Reorganization With Intramolecular Tunneling Of H-Atom: Formic Acid In Ar Matrix  
 J. Chem. Phys., 2009, 130, 144502.
295. Gu X., Zhang F., Kaiser R.I., Kislov V.V., Mebel A.M.  
 Reaction dynamics of the phenyl radical with 1,2-butadiene  
 Chem. Phys. Lett., 2009, 474, 51-56.
296. Zyubin A.S., Mebel A.M., Hayashi M., Chang H.C., Lin S.H.  
 Quantum chemical modeling of photo-absorption properties of the two- and three- nitrogen-vacancy point defects in diamond  
 J. Phys. Chem. C, 2009, 113, 10432-10440.
297. Zhang F., Kim Y.S., Kaiser R.I., Jamal A., Mebel A.M.  
 A Crossed Beams and Ab Initio Investigation on the Synthesis of Cyanodiacetylene under Single Collision Conditions - A Key Molecule in Extraterrestrial Chemistry  
 J. Chem. Phys., 2009, 130, 234308 (8 pp.).
298. Wang Q., Wu D., Zhang D., Jin M., Liu F., Liu H., Hu Z., Ding D., Mineo H., Dyakov Y., Teranishi Y., Chao S.D., Mebel A.M., Lin S.H.  
 Ionization and Dissociation Processes of Pyrrolidine in Intense Femtosecond laser Field  
 J. Phys. Chem. C, 2009, 113, 11805-11815.
297. Gu X., Kaiser R.I., Mebel A.M., Kislov V.V., Klippenstein S.J., Harding L.B., Liang M.C., Yung Y.L.  
 Cyanoethynyl Radical in Titan's Atmosphere  
 Astrophys. J., 2009, 701, 1797-1803.
299. Mebel A.M., Kislov V.V.  
 Can the  $C_5H_5 + C_5H_5 \rightarrow C_{10}H_{10} \rightarrow C_{10}H_9 + H / C_{10}H_8 + H_2$  Reaction Produce Naphthalene? An ab initio/RRKM study  
 J. Phys. Chem. A, 2009, 113, 9825-9833.
300. Gu X., Kim Y.S., Kaiser R.I., Mebel A.M., Liang M.C., Yung Y.L.

Chemical Dynamics of Triacetylene Formation and Application to Titan's Atmosphere

Proc . Nat. Acad. Sci., 2009, 106, 16078-16083.

301. Zhou C.-W., Mebel A.M., Li X.-Y.  
An ab initio/Rice-Ramsperger-Kassel-Marcus Study of the Reactions of Propenols with OH. Mechanism and Kinetics of H Abstraction Channels  
J. Phys. Chem. A, 2009, 113, 10667-10677.
303. Krishtal S.P., Mebel A.M., Kaiser R.I.  
A Theoretical Study of the Reaction Mechanism and Product Branching Ratios of  $C_2H + C_2H_4$  and Related Reactions on the  $C_4H_5$  Potential Energy Surface  
J. Phys. Chem. A, 2009, 113, 11112–11128.
304. Zhang F., Kim Y.S., Kaiser R.I., Krishtal S.P., Mebel A.M.  
A Crossed Molecular Beams Study on the Formation of Vinylacetylene in Titan's Atmosphere  
J. Phys. Chem. A, 2009, 113, 11167–11173.
305. Silva R., Gichuhi W.K., Kislov V.V., Landera A., Mebel A.M., Suits A.G.  
The UV photodissociation of cyanoacetylene: a combined ion imaging and theoretical investigation  
J. Phys. Chem. A, 2009, 113, 11182–11186.
306. Kaiser R.I., Zhang F., Gu X., Kislov V.V., Mebel A.M.  
Reaction Dynamics of the Phenyl Radical ( $C_6H_5$ ) with 1-Butyne ( $HCCC_2H_5$ ) and 2-Butyne ( $CH_3CCCH_3$ )  
Chem. Phys. Lett., 2009, 481, 46-53.
307. Yao L., Mebel A.M., Lin S.H.  
Dissociation Rate Constant of the Hydrogen Fluoride Dimer by the ab initio Anharmonic RRKM Theory  
J. Phys. Chem. A, 2009, 113, 14664-14669.
308. Landrum J.T., Chatfield D.C., Mebel A.M. I, Alvarez-Calderon F., Fernandez M.V.  
The conformation of end-groups is one determinant of carotenoid topology suitable for high fidelity molecular recognition: A study of  $\beta$ - and  $\epsilon$ -end-groups  
Arc. Biochem Biophys., 2010, 493, 169-174.
309. Kaiser R.I., Mebel A.M., Kostko O., Ahmed M.  
On the Ionization Energies of  $C_4H_3$  Isomers  
Chem. Phys. Lett., 2010, 485, 281-285.
310. Zhang F., Jones B., Maksyutenko P., Kaiser R.I., Chin C., Kislov V.V., Mebel A.M.  
Formation of the Phenyl Radical [ $C_6H_5(X^2A_1)$ ] under Single Collision Conditions – A Crossed Molecular Beam and Ab Initio Study  
J. Am. Chem. Soc., 2010, 132, 2672-2683.
311. Christiansen C.J., Dalal S.S., Francisco J.S., Mebel A.M., Gaffney J.S.

- Hydroxyl Radical Substitution in Halogenated Carbonyls: Oxalic Acid Formation  
J. Phys. Chem. A, 2010, 114, 2806-2820.
312. Jamal A., Mebel A.M.  
An Ab Initio/RRKM Study of the Reaction Mechanism and Product Branching Ratios of the Reactions of Ethynyl Radical with Allene and Methylacetylene  
Phys. Chem. Chem. Phys., 2010, 12, 2606-2618.
313. Jones B., Zhang F., Maksyutenko P., Mebel A.M., Kaiser R.I.  
A Crossed Molecular Beam Study on the Formation of Phenylacetylene and Its Relevance to Titan's Atmosphere  
J. Phys. Chem. A, 2010, 114, 5256-5262.
314. Huang C., Zhang F., Kaiser R.I., Kislov V.V., Mebel A.M., Silva R., Gichuhi W.K., Suits A.G.  
Photodissociation of diacetylene dimer and implications for hydrocarbon growth in Titan's atmosphere  
Astrophys. J., 2010, 714, 1249-1255.
315. Sebree J.A., Kislov V.V., Mebel A.M., Zwier T.S.  
Spectroscopic and Thermochemical Consequences of site-specific H-atom addition to Naphthalene  
J. Phys. Chem. A, 2010, 114, 6255-6262.
316. Zhou L., Zheng W., Kaiser R.I., Landera A., Mebel A.M., Liang M.-C., Yung Y.L.  
Cosmic-Ray Mediated Formation of Benzene on the Surface of Saturn's Moon Titan  
Astrophys. J., 2010, 718, 1243-1251.
317. Kislov V.V., Mebel A.M.  
Ab Initio/RRKM-ME Study on the Mechanism and Kinetics of the Reaction of Phenyl Radical with 1,2-Butadiene  
J. Phys. Chem. A, 2010, 114, 7682-7692.
318. Kaiser R.I., Sun B.J., Lin H.M., Chang A.H.H., Mebel A.M., Kostko O., Ahmed M.  
An Experimental and Theoretical Study on the Ionization Energies of Polyynes ( $H-(C\equiv C)_n-H$ ;  $n = 1-9$ )  
Astrophys. J., 2010, 719, 1884-1889.
319. Zhang F., Maksyutenko P., Kaiser R.I., Mebel A.M., Gregusova A., Perera A., Bartlett R.J.  
On the Gas Phase Synthesis of the Imidoborane Molecule (HNBH) via the Crossed Beam Reaction of Ground State Boron Atoms with Ammonia  
J. Phys. Chem. A, 2010, 114, 12148-12154.
320. Sebree J.A., Kislov V.V., Mebel A.M., Zwier T.S.

- Isomer Specific Spectroscopy of C<sub>10</sub>H<sub>n</sub>, n = 8-12: Exploring Pathways to Naphthalene in Titan's Atmosphere  
Faraday Disc., 2010, 147, 231-249.
321. Kaiser R.I., Maksyutenko P., Ennis C., Zhang F., Gu X., Krishtal S.P., Mebel A.M., Kostko O., Ahmed M.  
Untangling the Chemical Evolution of Titan's Atmosphere and Surface – From Homogeneous to Heterogeneous Chemistry  
Faraday Disc., 2010, 147, 429-478.
322. Landera A., Mebel A.M.  
Mechanisms of Formation of Nitrogen-Containing Polycyclic Aromatic Compounds in Low-Temperature Environments of Planetary Atmospheres: A Theoretical Study  
Faraday Disc., 2010, 147, 479-494.
323. Trakhtenberg L.I., Fokeyev A.A., Zyubin A.S., Mebel A.M., Lin S.H.  
Effect of Medium on Intramolecular H-atom Tunneling: Formic Acid Cis – Trans Conversion in Solid Matrices of Noble Gases  
J. Phys. Chem. B, 2010, 114, 17102-17112.
324. Gichuhi W.K., Mebel A.M., Suits A.G.  
UV Photodissociation of Ethylamine Cation: A Combined Experimental and Theoretical Investigation  
J. Phys. Chem. A, 2010, 114, 13296-13302.
325. Sivaraman B., Mebel A.M., Mason N.J., Babikov D., Kaiser R.I.  
On the Electron Induced Isotope Fractionation in Low Temperature <sup>32</sup>O<sub>2</sub>/<sup>36</sup>O<sub>2</sub> ices – Ozone as a Case Study  
Phys. Chem. Chem. Phys., 2011, 13, 421-427.
326. Jones B.M., Zhang F., Kaiser R.I., Jamal A., Mebel A.M., Cordiner M.A., Charnley S.B.  
Formation of Benzene in the Interstellar Medium  
Proc. Nat. Acad. Sci., 2011, 108, 452-457.
327. Landera A., Kaiser R.I., Mebel A.M.  
Addition of One and Two Units of C<sub>2</sub>H to Styrene: A Theoretical Study of the C<sub>10</sub>H<sub>9</sub> and C<sub>12</sub>H<sub>9</sub> Systems and Implications towards Growth of Polycyclic Aromatic Hydrocarbons at Low Temperatures  
J. Chem. Phys., 2011, 134, 024302 (13 pp.) .
328. Parker D.S.N., Zhang F., Kim, Y.S. Kaiser R.I., Mebel A.M.  
On the Formation of Resonantly Stabilized C<sub>5</sub>H<sub>3</sub> Radicals -A Crossed Beam and Ab Initio Study of the Reaction of Ground State Carbon Atoms with Vinylacetylene  
J. Phys. Chem. A, 2011, 115, 593-601.
329. Jamal A. Mebel A.M.  
Reactions of C<sub>2</sub>H with 1- and 2-Butynes: An Ab Initio/RRKM Study of the Reaction Mechanism and Product Branching Ratios

- J. Phys. Chem. A, 2011, 115, 2196-2207.
330. Zhang F., Parker D., Kim, Y.S. Kaiser R.I., Mebel A.M.  
On the Formation of Ortho-Benzyne (*o*-C<sub>6</sub>H<sub>4</sub>) under Single Collision  
Conditions and Its Role in Interstellar Chemistry  
Astrophys. J., 2011, 728, 141 (10 pp.).
331. Zhang F., Kaiser R.I., Kislov V.V., Mebel A.M., Golan A., Ahmed M.  
A VUV Photoionization Study of the Formation of the Indene Molecule and Its  
Isomers  
J. Phys. Chem. Lett., 2011, 2, 1731-1735.
332. Kaiser R.I., Goswami M., Maksyutenko P., Zhang F., Kim Y.S., Landera A.,  
Mebel A.M.  
A Crossed Molecular Beams and Ab Initio Study on the Formation of C<sub>6</sub>H<sub>3</sub>  
Radicals - An Interface between Resonantly Stabilized (RSFRs) and Aromatic  
Radicals (ARs)  
J. Phys. Chem. A., 2011, 115, 10251-10258.
333. Wnuk S.F., Penjarla J.A.K., Dang T., Mebel A.M., Nauser T., Schoeneich C.  
Modeling of the Ribonucleotide Reductases Substrate Reaction. Hydrogen  
Atom Abstraction by a Thiyl Free Radical and Detection of the Ribosyl-based  
Carbon Radical by Pulse Radiolysis  
Col. Czech. Chem. Com., 2011, 76, 1223-1238.
334. Morales S.B., Bennett C.J., Le Picard S.D., Canosa A., Sims I.R., Sun B.J.,  
Chen P.H., Chang A.H.H., Kislov V.V., Mebel A.M., Gu X., Zhang F., Kaiser  
R.I.  
A Crossed Molecular Beam, Low-Temperature Kinetics, and Theoretical  
Investigation of the Reaction of the Cyano Radical (CN) with 1,3-Butadiene  
(C<sub>4</sub>H<sub>6</sub>). A Route to Complex Nitrogen-Bearing Molecules in Low-Temperature  
Extraterrestrial Environments  
Astrophys. J., 2011, 742, 26 (10 pp.).
335. Parker D.S.N., Zhang F., Kaiser R.I., Kislov V.V., Mebel A.M.  
Indene Formation under Single Collision Conditions from Reaction of Phenyl  
Radicals with Allene and Phenylacetylene – A Crossed Molecular Beam and  
Ab Initio Study  
Chem. Asian J., 2011, 6, 3035-3042.
336. Jamal A., Mebel A.M.  
An Ab Initio/RRKM Study of the Reaction Mechanism and Product Branching  
Ratios of the Reactions of Ethynyl Radical with 1,2-Butadiene  
Chem. Phys. Lett., 2011, 518, 29-37.
337. Kaiser R.I., Goswami M., Zhang F., Parker D., Kislov V.V., Mebel A.M.,  
Aguilera-Iparraguirre J., Green W.H.

- Crossed Beam Reaction of Phenyl and D5-Phenyl Radicals with Propene and Deuterated Counterparts – Competing Atomic Hydrogen and Methyl Loss Pathways  
 Phys. Chem. Chem. Phys., 2012, 14, 720-729.
338. Parker D.S.N., Zhang F., Kaiser R.I., Landera A., Kislov V.V., Mebel A.M., Tielens A.G.G.M.  
 Low Temperature Formation of Naphthalene and its Role in the Synthesis of PAH in the Interstellar Medium  
 Proc. Nat. Acad. Sci., 2012, 109, 53-58.
339. Parker D.S.N., Zhang F., Kim Y.S., Kaiser R.I., Landera A., Mebel A.M.  
 On the Formation of Phenylacetylene (C<sub>6</sub>H<sub>5</sub>CCCCH) and D5-Phenylacetylene (C<sub>6</sub>D<sub>5</sub>CCCCH) Studied under Single Collision Conditions  
 Phys. Chem. Chem. Phys., 2012, 14, 2997-3003.
340. Zhou C.-W., Kislov V.V., Mebel A.M.  
 The Reaction Mechanism of Naphthyl Radicals with Molecular Oxygen. I. A Theoretical Study of the Potential Energy Surface  
 J. Phys. Chem. A, 2012, 116, 1571-1585.
341. Kislov V.V., Mebel A.M., Aguilera-Iparraguirre J., Green W.H.  
 The Reaction of Phenyl Radical with Propylene as a Possible Source of Indene and Other Polycyclic Aromatic Hydrocarbons: An Ab Initio/RRKM-ME Study  
 J. Phys. Chem. A, 2012, 116, 2012, 4176-4191.
342. Kaiser R.I., Parker D.S.N., Zhang F., Landera A., Kislov V.V., Mebel A.M.  
 PAH Formation under Single Collision Conditions - Reaction of Phenyl Radical and 1,3-Butadiene to Form 1,4-Dihydronaphthalene  
 J. Phys. Chem. A, 2012, 116, 4248-4258.
343. Mebel A.M., Landera A.  
 Product branching ratios in photodissociation of phenyl radical: A theoretical Ab initio/RRKM study  
 J. Chem. Phys., 2012, 136, 234305 (9 pp.).
344. Dang T.P., Sobczak A.J., Mebel A.M., Chatgililoglu C., Whuk S.F.  
 Investigation of Reactions Postulated to Occur During Inhibition of Ribonucleotide Reductases by 2'-Azido-2'-Deoxynucleotides  
 Tetrahedron, 2012, 68, 5655-5667.
345. Kaiser R.I., Mebel A.M.  
 On the Formation of Polyacetylenes and Cyanopolyacetylenes in Titan's Atmosphere and their Role in Astrobiology  
 Chem. Soc. Rev., 2012, 41, 5490-5501.
346. Parker D.S.N., Wilson A.V., Kaiser R.I., Labrador T., Mebel A.M.  
 Synthesis of the Silaisocyanoacetylene Molecule  
 J. Am. Chem. Soc., 2012, 134, 13896-13901.
347. Parker D.S.N., Wilson A.V., Kaiser R.I., Labrador T., Mebel A.M.

- Gas Phase Synthesis of the Silaisocyanoethylene Molecule ( $C_2H_3NSi$ )  
J. Org. Chem., 2012, 77, 8574-8580.
348. Holness H.K., Jamal A., Mebel A.M., Almirall J.R.  
Separation mechanism of chiral impurities, ephedrine and pseudoephedrine, found in amphetamine-type substances using achiral modifiers in the gas phase  
Anal. Bioanal. Chem., 2012, 404, 2407-2416.
349. Kaiser R.I., Krishtal S.P., Mebel A.M., Kostko O., Ahmed M.  
An Experimental and Theoretical Study on the Ionization Energies of  $SiC_2H_x$  ( $x = 0, 1, 2$ ) Isomers in the Interstellar Medium  
Astrophys. J., 2012, 761, 178 (7 pp.).
350. Kaiser R.I., Mebel A.M., Golan A., Ahmed M.  
A VUV Photoionization Study on the Formation of Primary and Secondary Products in the Reaction of the Phenyl Radical with 1,3-Butadiene under Combustion Relevant Conditions.  
Phys. Chem. Chem. Phys., 2013, 15, 341-347.
351. Jamal A., Mebel A.M.  
A Theoretical Investigation of the Mechanism and Product Branching Ratios of the Reactions of Cyano Radical with 1- and 2-Butynes and 1,2-Butadiene  
J. Phys. Chem. A, 2013, 117, 741-755.
352. Landera A., Mebel A.M.  
Low-Temperature Mechanisms for the Formation of Substituted Azanaphthalenes through Consecutive CN and  $C_2H$  Additions to Styrene and N-Methylenebenzenamine: A Theoretical Study  
J. Am. Chem. Soc., 2013, 135, 7251-7263.
353. Kislov V.V., Sadovnikov A.I., Mebel A. M.  
Formation Mechanism of Polycyclic Aromatic Hydrocarbons beyond the Second Aromatic Ring  
J. Phys. Chem. A, 2013, 117, 4794-4816.
354. Trakhtenberg L.I., Fokeyev A.A., Mebel A.M.  
H/D kinetic isotope effect in HCOOH cis-trans conversion of formic acid in noble gas matrices  
Chem. Phys. Lett., 2013, 574, 47-50.
355. Dangi B.B., Parker D.S.N., Kaiser R.I., Jamal A., Mebel A.M.  
A Combined Experimental and Theoretical Study on the Gas-Phase Synthesis of Toluene under Single Collision Conditions  
Angew. Chem., Int. Ed., 2013, 52, 7186-7189.
356. Parker D.S.N., Balucani N., Stranges D., Kaiser R.I., Mebel A.M.

- A Crossed Beam and ab Initio Investigation on the Formation of Boronyldiacetylene ( $\text{HCCCC}^{11}\text{BO}$ ;  $X^1\Sigma^+$ ) via the Reaction of the Boron Monoxide Radical ( $^{11}\text{BO}$ ;  $X^2\Sigma^+$ ) with Diacetylene ( $\text{C}_4\text{H}_2$ ;  $X^1\Sigma_g^+$ )  
*J. Phys. Chem. A*, 2013, 117, 8189-8198.
357. Dangi B.B., Maity S., Kaiser R.I., Mebel A.M.  
 A Combined Crossed Beam and Ab Initio Investigation of the Gas Phase Reaction of Dicarbon Molecules ( $\text{C}_2$ ;  $X^1\Sigma_g^+/a^3\Pi_u$ ) with Propene ( $\text{C}_3\text{H}_6$ ;  $X^1A'$ ): Identification of the Resonantly Stabilized Free Radicals 1- and 3-Vinylpropargyl  
*J. Phys. Chem. A*, 2013, 117, 11783–11793.
358. Wang Q., Dyakov Y.A., Wu D., Zhang D., Jin M., Liu F., Liu H., Hu Z., Ding D., Mineo H., Teranishi Y., Chao S.D., Lin S.H., Kosheleva O.K., Mebel, A. M.  
 Ionization/dissociation processes of methyl-substituted derivatives of cyclopentanone in intense femtosecond laser field  
*Chem. Phys. Lett.*, 2013, 586, 21–28.
359. Parker D.S.N., Dangi B.B., Balucani N., Stranges D., Mebel A.M., Kaiser R.I.  
 Gas-Phase Synthesis of Phenyl Oxoborane ( $\text{C}_6\text{H}_5\text{BO}$ ) via the Reaction of Boron Monoxide with Benzene  
*J. Org. Chem.*, 2013, 78, 11896–11900.
360. Parker D.S.N., Yang T., Kaiser R.I., Landera A., Mebel A.M.  
 On the formation of ethynylbiphenyl ( $\text{C}_{14}\text{D}_5\text{H}_5$ ;  $\text{C}_6\text{D}_5\text{C}_6\text{H}_4\text{CCH}$ ) isomers in the reaction of D5-phenyl radicals ( $\text{C}_6\text{D}_5$ ;  $X^2A_1$ ) with phenylacetylene ( $\text{C}_6\text{H}_5\text{C}_2\text{H}$ ;  $X^1A_1$ ) under single collision conditions  
*Chem. Phys. Lett.*, 2014, 595-596, 230-236.
361. Parker D.S.N., Mebel A.M., Kaiser R.I.  
 The role of isovalency in the reactions of the cyano (CN), boron monoxide (BO), silicon nitride (SiN), and ethynyl ( $\text{C}_2\text{H}$ ) radicals with unsaturated hydrocarbons acetylene ( $\text{C}_2\text{H}_2$ ) and ethylene ( $\text{C}_2\text{H}_4$ )  
*Chem. Soc. Rev.*, 2014, 43, 2701-2713.
362. Dangi B.B., Parker D.S.N., Yang T., Kaiser R.I., Mebel A.M.  
 Gas-Phase Synthesis of the Benzyl Radical ( $\text{C}_6\text{H}_5\text{CH}_2$ )  
*Angew. Chem., Int. Ed.*, 2014, 53, 4608 –4613.
363. Joalland B., Shi Y., Kamasah A., Suits A.G., Mebel A.M.  
 Roaming Dynamics in Radical Addition-Elimination Reactions  
*Nature Communications*, 2014, 5, Article number: 4064,  
 doi:10.1038/ncomms5064
364. Yang T., Parker D.S.N., Dangi B.B., Kaiser R.I., Stranges D., Su Y.H., Chen S.-Y., Chang A.H.H., Mebel A.M.  
 Directed Gas Phase Formation of the Ethynylsulfidoboron Molecule ( $\text{HCCBS}$ )  
*J. Am. Chem. Soc.*, 2014, 136, 8387-8392.
365. Parker D.S.N., Maity S., Dangi B.B., Kaiser R.I., Landera A., Mebel A.M.

- Understanding the Chemical Dynamics of the Reactions of Dicarbon with 1-Butyne, 2-Butyne, and 1,2-Butadiene – Toward the Formation of Resonantly Stabilized Free Radicals  
Phys. Chem. Chem. Phys., 2014, 16, 12150-12163.
366. Yang T., Parker D.S.N., Dangi B.B., Kaiser R.I., Kislov V.V., Mebel A.M.  
Crossed Beam Reactions of the Phenyl ( $C_6H_5$ ;  $X^2A_1$ ) and D5-Phenyl Radical ( $C_6D_5$ ;  $X^2A_1$ ) with 1,2-Butadiene ( $H_2CCCHCH_3$ ;  $X^1A'$ )  
J. Phys. Chem. A, 2014, 118, 4372-4381.
367. Dangi B.B., Parker D.S.N., Kaiser R.I., Belisario-Lara D., Mebel A.M.  
An Experimental and Theoretical Investigation of the Formation of  $C_7H_7$  Isomers in the Bimolecular Reaction of Dicarbon Molecules with 1,3-Pentadiene  
Chem. Phys. Lett., 2014, 607, 92-99.
368. Dangi B.B., Yang T., Kaiser R.I., Mebel A.M.  
Reaction Dynamics of the 4-Methylphenyl Radical ( $C_6H_4CH_3$ ; p-Tolyl) with Isoprene ( $C_5H_8$ ) - Formation of Dimethyldihydronaphthalenes  
Phys. Chem. Chem. Phys., 2014, 16, 16805-16814.
369. Kaiser R.I., Dangi B.B., Yang T., Parker D.S.N., Mebel A.M., Korte A., Sander W.  
Reaction Dynamics of the 4-Methylphenyl Radical (p-Tolyl) with 1,2-Butadiene (1-Methylallene) – Are Methyl Groups purely Spectators?  
J. Phys. Chem. A, 2014, 118, 6181-6190.
370. Ribeiro J.M., Mebel A.M.  
Reaction Mechanism and Product Branching Ratios of the  $CH + C_3H_8$  Reaction: A Theoretical Study  
J. Phys. Chem. A, 2014, 118, 9080-9086.
371. Joalland B., Shi Y., Estillore A., Kamasah A., Mebel A.M., Suits A.G.  
Dynamics of Chlorine Atom Reactions with Hydrocarbons: Insights from Imaging the Radical Product in Crossed Beams (Feature Article)  
J. Phys. Chem. A 2014, 118, 9281-9295.
372. Kislov V.V., Singh R.I., Edwards D.E, Mebel A.M., Frenklach M.  
Rate coefficients and product branching ratios for the oxidation of phenyl and naphthyl radicals: A theoretical RRKM-ME study  
Proc. Int. Combust. Inst., 2015, 35, 1861-1869.
373. Yang T., Muzangwa, L., Parker D.S.N., Kaiser R.I., Mebel A.M.  
Formation of 2-and 1-methyl-1,4-dihydronaphthalene isomers via the crossed beam reactions of phenyl radicals ( $C_6H_5$ ) with isoprene ( $CH_2C(CH_3)CHCH_2$ ) and 1,3-pentadiene ( $CH_2CHCHCHCH_3$ )  
Phys. Chem. Chem. Phys., 2015, 17, 530-540.
374. Muzangwa L.G., Yang, T., Parker D.S.N., Kaiser R.I., Mebel A.M., Jamal A., Ryazantsev M., Morokuma K.

- A crossed molecular beam and ab initio study on the formation of 5-and 6-methyl-1,4-dihydronaphthalene (C<sub>11</sub>H<sub>12</sub>) via the reaction of meta-tolyl (C<sub>7</sub>H<sub>7</sub>) with 1,3-butadiene (C<sub>4</sub>H<sub>6</sub>)  
Phys. Chem. Chem. Phys. 2015, 17, 7699-7706.
375. Kaiser R.I., Parker D.S.N., Mebel A.M.  
Reaction dynamics in astrochemistry: low-temperature pathways to polycyclic aromatic hydrocarbons in the interstellar medium.  
Ann. Rev. Phys. Chem., 2015, 66, 43-67.
376. Yang T., Parker D.S.N., Dangi B.B., Kaiser R.I., Mebel A.M.  
Formation of 5- and 6-methyl-1H-indene (C<sub>10</sub>H<sub>10</sub>) via the reactions of the para-tolyl radical (C<sub>6</sub>H<sub>4</sub>CH<sub>3</sub>) with allene (H<sub>2</sub>CCCH<sub>2</sub>) and methylacetylene (HCCCH<sub>3</sub>) under single collision conditions  
Phys. Chem. Chem. Phys. 2015, 17, 10510-10519.
377. Parker D.S.N., Kaiser R.I., Kostko O., Troy T.P., Ahmed M., Mebel A.M., Tielens A.G.G.M.  
Gas Phase Synthesis of (Iso)Quinoline and Its Role in the Formation of Nucleobases in the Interstellar Medium  
Astrophys. J., 2015, 803, 53.
378. Ribeiro J.M., Mebel A.M.  
Reaction mechanism and rate constants of the CH+CH<sub>4</sub> reaction: a theoretical study  
Mol. Phys. 2015, 113, 1865-1872.
379. Parker D.S.N., Kaiser R.I., Troy T.P., Kostko O., Ahmed M., Mebel A.M.  
Toward the Oxidation of the Phenyl Radical and Prevention of PAH Formation in Combustion Systems  
J. Phys. Chem. A 2015, 119, 7145-7154.
380. Singh R.I., Mebel A.M., Frenklach M.  
Oxidation of Graphene-edge Six- and Five-member Rings by Molecular Oxygen  
J. Phys. Chem. A 2015, 119, 7528-7547.
381. Mebel A.M., Kaiser R.I.  
Formation of Resonantly Stabilised Free Radicals via the Reactions of Atomic Carbon, Dicarbon, and Tricarbon with Unsaturated Hydrocarbons: Theory and Crossed Molecular Beams Experiments  
Int. Rev. Phys. Chem. 2015, 34, 461-514.
382. Zagidullin M.V., Pershin A.A., Azyazov V.N., Mebel A. M.  
Luminescence of the (O<sub>2</sub>(a<sup>1</sup>Δ<sub>g</sub>))<sub>2</sub> collisional complex in the temperature range of 90-315 K: Experiment and theory  
J. Chem. Phys. 2015, 143, 244315 (13 pp.).
383. Azyazov V.N., Bresler S.M., Torbin A.P., Mebel A.M., Heaven M.C.  
Removal of Rb(6<sup>2</sup>P) by H<sub>2</sub>, CH<sub>4</sub>, and C<sub>2</sub>H<sub>6</sub>  
Optics Lett. 2016, 41, 669-672.

384. Ribeiro J.M., Mebel A.M.  
Reaction mechanism and product branching ratios of the CH + C<sub>3</sub>H<sub>6</sub> reaction:  
A theoretical study  
J. Phys. Chem. A 2016, 120, 1800-1812.
385. Forstel M., Maksyutenko P., Mebel A. M., Kaiser R.I.  
Pentacarbon dioxide (C<sub>5</sub>O<sub>2</sub>) formation and its role as a tracer of Solar System  
evolution  
Astrophys. J. Lett. 2016, 818, L30.
386. Forstel M., Tsegaw Y.A., Maksyutenko P., Mebel A.M., Sander W., Kaiser R.I.  
On the Formation of N<sub>3</sub>H<sub>3</sub> Isomers in Irradiated Ammonia Bearing Ices:  
Triazene (H<sub>2</sub>NNNH) or Triimide (HNHNNH)  
ChemPhysChem 2016, 17, 2726-2735.
387. Yang T., Troy T.P., Xu B., Kostko O., Ahmed M., Mebel A.M., Kaiser R.I.  
Hydrogen-Abstraction/Acetylene-Addition Exposed  
Angew. Chem. Int. Ed. 2016, 55, 14983-14987.
388. Benigni P., Bravo C., Quirke J.M.E., DeBord J.D., Mebel A.M., Fernandez-  
Lima, F.  
Analysis of Geologically Relevant Metal Porphyrins Using Trapped Ion  
Mobility Spectrometry Mass Spectrometry and Theoretical Calculations  
Energy & Fuels, 2016, 30, 10341-10347.
389. Thomas A.M., Yang T., Dangi B.B., Kaiser R.I., Kim G.S., Mebel A.M.  
Oxidation of the para-Tolyl Radical by Molecular Oxygen under Single-  
Collision Conditions: Formation of the para-Toloxyl Radical  
J. Phys. Chem. Lett. 2016, 24, 5121-5127.
390. Mebel A.M., Georgievskii Y., Jasper A.W., Klippenstein S.J.  
Pressure-dependent rate constants for PAH growth: formation of indene and  
its conversion to naphthalene  
Faraday Discuss. 2016, 195, 637-670.
391. Mebel A.M., Georgievskii Y., Jasper A.W., Klippenstein S.J.  
Temperature- and Pressure-Dependent Rate Coefficients for the HACA  
Pathways from Benzene to Naphthalene  
Proc. Combust. Inst. 2017, 36, 919-926.
392. Mebel A.M., Landera A., Kaiser R.I.  
Formation Mechanisms of Naphthalene and Indene: From the Interstellar  
Medium to Combustion Flames  
J. Phys. Chem. A 2017, 121, 901–926.
393. Zhao L., Yang T., Kaiser R.I., Troy T.P., Ahmed M., Belisario-Lara D., Ribeiro  
J.M., Mebel A.M.  
Combined Experimental and Computational Study on the Unimolecular  
Decomposition of JP-8 Jet Fuel Surrogates. I. *n*-Decane (*n*-C<sub>10</sub>H<sub>22</sub>)  
J. Phys. Chem. A 2017, 121, 1261–1280.

394. Zhao L., Yang T., Kaiser R.I., Troy T.P., Ahmed M., Ribeiro J.M., Belisario-Lara D., Mebel A.M.  
Combined Experimental and Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates. II: *n*-Dodecane (*n*-C<sub>12</sub>H<sub>26</sub>)  
J. Phys. Chem. A 2017, 121, 1281–1297.
395. Yang T., Kaiser R.I., Troy T.P., Xu B., Kostko O., Ahmed M., Mebel A.M., Zagidullin M.V., Azyazov V.N.  
HACA's Heritage: A Free Radical Pathway to Phenanthrene in Circumstellar Envelopes of Asymptotic Giant Branch Stars  
Angew. Chem. Int. Ed. 2017, 56, 4515-4519.
396. Azyazov V.N., Torbin A.P., Mebel A.M., Bresler S.M., Heaven M.C.  
Product channels of the reactions of Rb(6<sup>2</sup>P) with H<sub>2</sub>, CH<sub>4</sub> and C<sub>2</sub>H<sub>6</sub>  
J. Quant. Spectrosc. Rad. Trans. 2017, 196, 46-52.
397. Ghildina A.R., Oleinikov A.D., Azyazov V.N., Mebel A.M.  
Reaction Mechanism, Rate Constants, and Product Yields for Unimolecular and  
H-assisted Decomposition of 2,4-Cyclopentadienone and Oxidation of Cyclopentadienyl with Atomic Oxygen  
Combust. Flame, 2017, 183, 181-193.
398. Ribeiro J.M., Mebel A.M.  
Reaction Mechanism and Product Branching Ratios of The CH + C<sub>3</sub>H<sub>4</sub> Reactions: A Theoretical Study  
Phys. Chem. Chem. Phys., 2017, 19, 14543-14554.
399. Zhao L., Yang T., Kaiser R.I., Troy T.P., Xu B., Ahmed M., Alarcon J., Belisario-Lara D., Mebel A.M., Zhang Y., Cao C.  
A Vacuum Ultraviolet Photoionization Study on High-Temperature Decomposition of JP-10 (exo-Tetrahydrodicyclopentadiene)  
Phys. Chem. Chem. Phys., 2017, 19, 15780-15807.
400. Thomas A.M., Lucas M., Yang T., Kaiser R.I., Fuentes L., Belisario-Lara D., Mebel A.M.  
A Free-Radical Pathway to Hydrogenated Phenanthrene in Molecular Clouds  
—  
Low Temperature Growth of Polycyclic Aromatic Hydrocarbons  
ChemPhysChem, 2017, 18, 1971-1976.
401. Semenikhin A.S., Savchenkova A.S., Chechet I.V., Matveev S.G., Liu Z., Frenklach M., Mebel A.M.  
Rate constants for H abstraction from benzo(a)pyrene and chrysene: a theoretical study  
Phys. Chem. Chem. Phys., 2017, 19, 25401-25413.
402. Zagidullin M.V., Khvatov N.A., Medvedkov I.A., Tolstov G.I., Mebel A.M., Heaven

- M.C., Azyazov V.N.  
O<sub>2</sub>(b<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) quenching by O<sub>2</sub>, CO<sub>2</sub>, H<sub>2</sub>O, and N<sub>2</sub> at temperatures of 300-800 K  
J. Phys. Chem. A, 2017, 121, 7343-7348.
403. Cui D., Mebel A.M., Arroyo-Mora L.E., Holness H., Furton K.G., O'Shea K.  
Kinetic, product, and computational studies of the ultrasonic induced degradation  
of 4-methylcyclohexanemethanol (MCHM)  
Water Research, 2017, 126, 164-171.
404. Lucas M., Zhao L., Thomas A.M., Kaiser R.I., Kim G.-S., Mebel A.M.  
Gas Phase Synthesis of the Elusive Cyclooctatetraenyl Radical (C<sub>8</sub>H<sub>7</sub>) via Triplet  
Aromatic Cyclooctatetraene (C<sub>8</sub>H<sub>8</sub>) and Non-Aromatic Cyclooctatriene (C<sub>8</sub>H<sub>8</sub>) Intermediates  
Angew. Chem., Int. Ed., 2017, 56, 13655-13660.
405. Krasnoukhov V.S., Porfiriev D.P., Zavershinskiy I.P., Azyazov V.N., Mebel A.M.  
Kinetics of the CH<sub>3</sub> + C<sub>5</sub>H<sub>5</sub> Reaction: A Theoretical Study  
J. Phys. Chem. A, 2017, 121, 9191-9200.
406. Jonah T.M., Mathivathanan L., Morozov A.N., Mebel A.M., Raptis R.G., Kavallieratos K.  
Remarkably selective NH<sub>4</sub><sup>+</sup> binding and fluorescence sensing by tripodal tris(pyrazolyl) receptors derived from 1,3,5-triethylbenzene: structural and theoretical insights on the role of ion pairing  
New J. Chem., 2017, 41, 14835-14838.
407. Galimova G.R., Azyazov V.N., Mebel A.M.  
Reaction mechanism, rate constants, and product yields for the oxidation of cyclopentadienyl and embedded five-member ring radicals with hydroxyl  
Combust. Flame, 2018, 187, 147-164.
408. Frenklach M., Liu Z., Singh R.I., Galimova G.R., Azyazov V.N., Mebel A.M.  
Detailed, sterically-resolved modeling of soot oxidation: role of o atoms, interplay  
with particle nanostructure, and emergence of inner particle burning  
Combust. Flame, 2018, 188, 284-306.
409. Yang M., Sun Y., Zhang X., McCord B., McGoron A.J., Mebel A., Cai Y.  
Raman spectra of thiolated arsenicals with biological importance  
Talanta, 2018, 179, 520-530.
410. Torbin A.P., Pershin A.A., Mebel A.M., Zagidullin M.V., Heaven M.C., Azyazov V.N.  
Collisional relaxation of O<sub>2</sub>(a<sup>1</sup>Δ, u = 1, 2, 3) by CO<sub>2</sub>  
Chem. Phys. Lett. 2018, 691, 456-461.

411. Oleinikov A.D., Azyazov V.N., Mebel A.M.  
Oxidation of Cyclopentadienyl Radical with Molecular Oxygen: A Theoretical Study  
Combust. Flame, 2018, 191, 309-319.
412. Semenikhin A.S., Shubina E.G., Savchenkova A.S., Chechet I.V., Matveev S.G.,  
Konnov A.A., Mebel A.M.  
Mechanism and Rate Constants of the CH<sub>3</sub> + CH<sub>2</sub>CO Reaction: A Theoretical Study  
Int. J. Chem. Kinet., 2018, 50, 273-284.
413. Yang T., Thomas A.M., Dangi B.B., Kaiser R.I., Mebel A.M., Millar T.J.  
Low temperature synthesis of silicon oxides and their potential role in the formation of interstellar silicates  
Nature Commun., 2018, 9, 774.
414. Lucas M., Thomas A.M., Kaiser R.I., Bashkirov E.K., Azyazov V.N., Mebel A.M.  
A Combined Experimental and Computational Investigation of the Elementary Reaction of Ground State Atomic Carbon (C; <sup>3</sup>P<sub>j</sub>) with Pyridine (C<sub>5</sub>H<sub>5</sub>N; X<sup>1</sup>A<sub>1</sub>) via Ring Expansion and Ring Degradation Pathways  
J. Phys. Chem. A, 2018, 122, 3128-3139.
415. Zhao L., Kaiser R.I., Xu B., Ablikim U., Ahmed M., Joshi D., Veber G., Fischer F.R., Mebel A.M.  
On the Synthesis of Pyrene in Circumstellar Envelopes and Its Role in the Formation of Two-Dimensional Nanostructures  
Nature Astron., 2018, 2, 403-419.
416. Thomas A.M., Lucas M., Zhao L., Liddiard J., Kaiser R.I., Mebel A.M.  
A Combined Crossed Molecular Beams and Computational Study on the Formation of Distinct Resonantly Stabilized C<sub>5</sub>H<sub>3</sub> Radicals via Chemically Activated C<sub>5</sub>H<sub>4</sub> and C<sub>6</sub>H<sub>6</sub> Intermediates  
Phys. Chem. Chem. Phys., 2018, 20, 10906-10925.
417. Belisario-Lara D., Mebel A.M., Kaiser R.I.  
Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates III: Butylbenzene Isomers (n-, s-, and t-C<sub>14</sub>H<sub>10</sub>)  
J. Phys. Chem. A, 2018, 122, 3980-4001.
418. Zhao L., Kaiser R.I., Xu B., Ablikim U., Ahmed M., Zagidullin M.V., Azyazov V.N., Howlader A.H., Wnuk S.F., Mebel A.M.  
A VUV Photoionization Study on the Formation of the Simplest Polycyclic Aromatic Hydrocarbon: Naphthalene (C<sub>10</sub>H<sub>8</sub>)  
J. Phys. Chem. Lett., 2018, 9, 2620-2626.
419. Morozov A.N., Govor E.V., Anagnostopoulos V.A., Kavallieratos K., Mebel A.M.

- 1,3,5-Tris-(4-(iso-propyl)-phenylsulfamoylmethyl)benzene as a potential Am(III) extractant: experimental and theoretical study of Sm(III) complexation and extraction and theoretical correlation with Am(III)  
Mol. Phys., 2018, 116, 2719-2727.
421. Morozov A.N., Mebel A.M., Kaiser R.I.  
A Theoretical Study of Pyrolysis of JP-10 (exo-Tetrahydrodicyclopentadiene) and its Primary and Secondary Unimolecular Decomposition Products  
J. Phys. Chem. A, 2018, 122, 4920–4934.
422. Zagidullin M.V., Khvatov N.A., G.I. Tolstov G.I., Medvedkov I.A., Mebel A.M., Heaven M.C., Azyazov V.N.  
O<sub>2</sub>(b<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) removal by H<sub>2</sub>, CO, N<sub>2</sub>O, CH<sub>4</sub> and C<sub>2</sub>H<sub>4</sub> in the 300–800 K temperature range  
J. Phys. Chem. A, 2018, 122, 5283–5288.
423. Ghildina A.R., Mebel A.M., Medvedkov I.A., Azyazov V.N.  
Quantum-Chemical Calculations of the Primary Reactions of Thermal Decomposition of Cyclopentadienone  
Combust. Expl. Shock Waves, 2018, 54, 9-15.
424. Lucas M., Thomas A.M., Yang T., Kaiser R.I., Mebel A.M., Hait D., Head-Gordon M.  
Unusual Chemistry in the Phenyl - Silane System: Exploring the Prototype of a Facile S<sub>R</sub>2 Reaction Mechanism  
J. Phys. Chem. Lett., 2018, 9, 5135–5142.
425. Thomas A.M., Zhao L., He C., Mebel A.M., Kaiser R.I.  
A Combined Experimental and Computational Study on the Reaction Dynamics of the 1-Propynyl (CH<sub>3</sub>CC)-Acetylene (HCCH) System and the Formation of Methylidyneacetylene (CH<sub>3</sub>CCCCH)  
J. Phys. Chem. A, 2018, 122, 6663-6672.
426. Zagidullin M.V., Kaiser R.I., Porfiriev D.P., Zavershinskiy I.P., Ahmed M., Azyazov V.N., Mebel A.M.  
Functional Relationships between Kinetic, Flow, and Geometrical Parameters in a High-Temperature Chemical Microreactor  
J. Phys. Chem. A, 2018, 122, 8819–8827.
427. Cui D.N., Mebel A.M., Arroyo-Mora L.E., Zhao C., De Caprio A., O'Shea K.  
Fundamental study of the ultrasonic induced degradation of the popular antihistamine, diphenhydramine (DPH)  
Water Research, 2018, 144, 265-273.
428. Zhao L., Kaiser R.I., Xu B., Ablikim U., Ahmed M., Evseev M.M., Bashkirov E.K., Azyazov V.N., Mebel A.M.  
Low-temperature formation of polycyclic aromatic hydrocarbons in Titan's atmosphere  
Nature Astron., 2018, 2, 973-979.
429. Pershin A.A., Torbin A.P., Zagidullin M.V., Mebel A.M., Mikheyev P.A., Azyazov

- V.N.  
Rate constants for collision-induced emission of  $O_2(a^1\Delta_g)$  with He, Ne, Ar, Kr,  $N_2$ ,  $CO_2$  and  $SF_6$  as collisional partners  
Phys. Chem. Chem. Phys., 2018, 20, 29677-29683.
430. Savchenkova A.S., Semenikhin A.S., Chechet I.V., Matveev S.G., Konnov A.A., Mebel A.M.  
Mechanism and rate constants of the  $CH_2 + CH_2CO$  reactions in triplet and singlet states: A theoretical study  
J. Comput. Chem., 2019, 40, 387–399.
431. Frenklach M., Singh R.I., Mebel A.M.  
On the low-temperature limit of HACA  
Proc. Combust. Inst., 2019, 37, 969-976.
432. Galimova G.R., Azyazov V.N., Porfiriev D.P., Mebel A.M.  
Reaction mechanism, rate constants, and product yields for the oxidation of embedded five-member ring radicals with atomic oxygen  
Chem. Phys., 2019, 519, 101-109.
433. Khvatov N.A., Zagidullin M.V., Tolstov G.I., Medvedkov I.A., Mebel A.M., Heaven M.C.; Azyazov V.N.  
Product channels of the reactions of  $O_2(b^1\Sigma_g^+)$   
Chem. Phys., 2019, 521, 85-91.
434. Deriu C., Conticello I., Mebel A.M., McCord B.  
Micro solid phase extraction surface-enhanced Raman spectroscopy ( $\mu$ -SPE /SERS) screening test for the detection of the synthetic cannabinoid JWH-018 in oral fluid  
Anal. Chem., 2019, 91, 4780-4789.
435. Zhao L., Bo X., Ablikim U., Lu W., Ahmed M., Evseev M.M., Bashkurov E.K., Azyazov V.N., Howlader A.H., Wnuk S.F., Mebel A.M., Kaiser R.I.  
Gas-Phase Synthesis of Triphenylene ( $C_{18}H_{12}$ )  
ChemPhysChem, 2019, 20, 791-797.
436. Morozov A.N., Mebel A.M.  
Theoretical Study of the Reaction Mechanism and Kinetics of the Phenyl + Allyl and Related Benzyl + Vinyl Associations  
J. Phys. Chem. A, 2019, 123, 1720-1729.
437. Thomas A.M., Dangi B.B., Yang T., Tarczay G., Kaiser R.I., Sun B.-J., Chen S.-Y., Chang A.H.H., Nguyen T.L., Stanton J.F., Mebel A.M.  
Directed Gas-Phase Formation of the Germaniumsilylene Butterfly Molecule ( $Ge(\mu-H_2)Si$ )  
J. Phys. Chem. Lett. 2019, 10, 1264-1271.

438. Zhao L., Kaiser R.I., Xu B., Ablikim U., Lu W., Ahmed M., Evseev M.M., Bashkirov E.K., Azyazov V.N., Zagidullin M. V., Morozov A.N., Howlader A.H., Wnuk S.F., Mebel A.M., Joshi D., Veber G., Fischer F.R.  
Gas phase synthesis of [4]-helicene  
Nature Comm. 2019, 10, 1510.
439. Ghildina A.R., Porfiriev D.P., Azyazov V.N., Mebel A.M.  
The Mechanism and Rate Constants for Oxidation of Indenyl Radical C<sub>9</sub>H<sub>7</sub> with Molecular Oxygen O<sub>2</sub>: A Theoretical Study  
Phys. Chem. Chem. Phys., 2019, 21, 8915-8924.
440. Zhao L., Prendergast M.B., Kaiser R.I., Xu B., Lu W., Ablikim U., Ahmed M., Oleinikov A.D., Azyazov V.N., Mebel A.M., Howlader A.H., Wnuk S.F.  
Reactivity of the Indenyl Radical (C<sub>9</sub>H<sub>7</sub>) with Acetylene (C<sub>2</sub>H<sub>2</sub>) and Vinylacetylene (C<sub>4</sub>H<sub>4</sub>)  
ChemPhysChem, 2019, 20, 1437-1447.
441. Kandel S., Veerasamy S., Mathivathanan L., Morozov A.N., Mebel A., Raptis R.  
Aggregation Induced Emission Enhancement (AIEE) of Tripodal Pyrazole Derivatives for Sensing of Nitroaromatics; Vapor Phase Detection of Picric Acid  
New J. Chem., 2019, 43, 7251-7258.
442. Thomas A.M., He C., Zhao L., Galimova G.R., Mebel A.M., Kaiser R.I.  
A Combined Experimental and Computational Study on the Reaction Dynamics of the 1-Propynyl (CH<sub>3</sub>CC) – 1,3-butadiene (CH<sub>2</sub>CHCHCH<sub>2</sub>) System and the Formation of Toluene under Single Collision Conditions  
J. Phys. Chem. A, 2019, 123, 4104-4118.
443. He C., Thomas A.M., Zhao L., Galimova G.R., Mebel A.M., Kaiser R.I.  
Gas Phase Formation of Methyltriacetylene (CH<sub>3</sub>(C≡C)<sub>3</sub>H) - An Interstellar Molecule  
ChemPhysChem, 2019, 20, 1912-1917.
444. He C., Zhao L., Thomas A.M., Morozov A.N., Mebel A.M., Kaiser R.I.  
On the Formation of Distinct C<sub>6</sub>H<sub>6</sub> Isomers under Single-Collision Conditions via the Reactions of the 1-Propynyl Radical (CH<sub>3</sub>CC; X<sup>2</sup>A<sub>1</sub>) with Methylacetylene (H<sub>3</sub>CCCH; X<sup>1</sup>A<sub>1</sub>) and Allene (H<sub>2</sub>CCCH<sub>2</sub>; X<sup>1</sup>A<sub>1</sub>)  
J. Phys. Chem. A, 2019, 123, 5446-5462.
445. Ghildina A.R., Porfiriev D.P., Azyazov V.N., Mebel A.M.  
Scission of the Five-Member Ring in 1-H-Inden-1-One C<sub>9</sub>H<sub>6</sub>O and Indenyl C<sub>9</sub>H<sub>7</sub> in the Reactions with H and O Atoms  
J. Phys. Chem. A, 2019, 123, 5741-5752.
446. Zhao L., Prendergast M., Kaiser R.I., Xu B., Ablikim U., Lu W., Ahmed M., Oleinikov A.D., Azyazov V.N., Howlader A.H., Wnuk S.F., Mebel A.M.

- How to add a five-membered ring to polycyclic aromatic hydrocarbons (PAHs)  
 — molecular mass growth of the 2-naphthyl radical ( $C_{10}H_7$ ) to benzindenes ( $C_{13}H_{10}$ ) as a case study  
 Phys. Chem. Chem. Phys., 2019, 21, 16737-16750.
447. Wang L., Deriu C., Wu W.S., Mebel A.M., McCord B.  
 Surface-enhanced Raman spectroscopy, Raman, and density functional theoretical analyses of fentanyl and six analogs  
 J. Raman Spectrosc., 2019, 50, 1405-1415.
448. Zhao L., Kaiser R.I., Lu W., Xu B., Ahmed M., Morozov A.N., Mebel A.M., Howlader A.H., Wnuk S.F.  
 Molecular Mass Growth through Ring Expansion in Polycyclic Aromatic Hydrocarbons via Radical-Radical Reactions  
 Nature Comm. 2019, 10, 3689.
449. Thomas A.M., Zhao L., He C., Galimova G.R., Mebel A.M., Kaiser R.I.  
 Directed Gas Phase Synthesis of Triafulvene under Single Collision Conditions  
 Angew. Chem., Int. Ed., 2019, 58, 15488-15495.
450. He C., Zhao L., Thomas A.M., Galimova G.R., Mebel A.M., Kaiser R.I.  
 A Combined Experimental and Computational Study on the Reaction Dynamics of the 1-Propynyl Radical ( $CH_3CC$ ;  $X^2A_1$ ) with Ethylene ( $H_2CCH_2$ ;  $X^1A_{1g}$ ) and the Formation of 1-Penten-3-yne ( $CH_2CHCCCH_3$ ;  $X^1A'$ )  
 Phys. Chem. Chem. Phys., 2019, 21, 22308-22319.
451. Zagidullin M.V., Khvatov N.A., Medvedkov I.A., Mebel A.M., Heaven M.C., Azyazov V.N.  
 $O_2(b^1\Sigma_g^+)$  removal by  $I_2$  and NO at temperatures of 297-750 K  
 Chem. Phys. Lett., 2019, 735, 136774.
452. He C., Thomas A.M., Galimova G.R., Mebel A.M., Kaiser R.I.  
 Gas-Phase Formation of 1-Methylcyclopropene and 3-Methylcyclopropene via the Reaction of the Methylidyne Radical ( $CH$ ;  $X^2\Pi$ ) with Propylene ( $CH_3CHCH_2$ ;  $X^1A'$ )  
 J. Phys. Chem. A, 2019, 123, 10543-10555.
453. Thomas A.M., Doddipatla S., Kaiser R.I., Galimova G.R., Mebel A.M.  
 A Barrierless Pathway Accessing the  $C_9H_9$  and  $C_9H_8$  Potential Energy Surfaces via the Elementary Reaction of Benzene with 1-Propynyl  
 Scientific Reports, 2019, 9, 17595.
454. Pershin A.A., Ghildina A.R., Mebel A.M., Azyazov V.N., Mikheyev P.A., Heaven M.C.  
 Computational investigation of energy transfer and line broadening for  $Ar^* + He$

- collisions  
J. Chem. Phys., 2019, 151, 224306.
455. Porfiriev D.P., Azyazov V.N., Mebel A.M.  
Conversion of Acenaphthalene to Phenalene via Methylation: A Theoretical Study  
Combust. Flame, 2020, 213, 302-313.
456. Mikheyev P.A., Demyanov A.V., Kochetov I.V., Sludnova A.A., Torbin A.P., Mebel A.M., Azyazov V.N.  
Ozone and oxygen atoms production in a dielectric barrier discharge in pure oxygen and O<sub>2</sub>/CH<sub>4</sub> mixtures. Modeling and experiment  
Plasma Sources Sci.Tech., 2020, 29, 015012.
457. He C., Thomas A.M., Galimova G.R., Morozov A.N., Mebel A.M., Kaiser R.I.  
Gas-Phase Formation of Fulvenallene (C<sub>7</sub>H<sub>6</sub>) via the Jahn-Teller Distorted Tropyli (C<sub>7</sub>H<sub>7</sub>) Radical Intermediate under Single-Collision Conditions  
J. Am. Chem. Soc., 2020, 142, 3205-3213.
458. Zhao L., Kaiser R.I., Xu B., Ablikim U., Ahmed M., Evseev M.M., Bashkirov E.K.,  
Azyazov V.N., Mebel A.M.  
A Unified Mechanism on the Formation of Acenes, Helicenes, and Phenacenes  
in the Gas Phase  
Angew. Chem., Int. Ed., 2020, 59, 4051-4058.
459. Frenklach M., Mebel A.M.  
On the mechanism of soot nucleation  
Phys. Chem. Chem. Phys., 2020, 22, 5314-5331.
460. Morozov A.N., Mebel A.M.  
Theoretical Study of the Reaction Mechanism and Kinetics of the Phenyl + Propargyl Association  
Phys. Chem. Chem. Phys., 2020, 22, 6868-6880.
461. Singh S.K., La Jeunesse J., Vuppuluri V., Son S.F., Sun B.-J., Chang A.H.H., Mebel A.M., Kaiser R.I.  
The Elusive Ketene (H<sub>2</sub>CCO) Channel in the Infrared Multiphoton Dissociation of Solid 1,3,5-Trinitro-1,3,5-Triazinane (RDX)  
ChemPhysChem, 2020, 21, 837-842.
462. Savchenkova A.S., Semenikhin A.S., Chechet I.V., Matveev S.G., Mebel A.M.,  
Konnov A.A.  
Revisiting diacetyl and acetic acid flames: the role of the ketene + OH reaction  
Combust. Flame, 2020, 218, 28-41.
463. Govor E.V., Morozov A.N., Rains A.A., Mebel A.M., Kavallieratos K.

Spectroscopic and Theoretical Insights into Surprisingly Effective Sm(III) Extraction from Alkaline Aqueous Media by *o*-Phenylenediamine-Derived Sulfonamides

Inorg. Chem., 2020, 59, 6884-6894.

464. Zhao L., Kaiser R.I., Lu W., Ahmed M., Evseev M.M., Bashkirov E.K., Azyazov V.N., Mebel A.M., Tönshoff C., Reicherter F., Bettinger H.F. A Free Radical Prompted Barrierless Gas Phase Synthesis of Pentacene Angew. Chem., Int. Ed., 2020, 59, 11334-11338.
465. He C., Zhao L., Doddipatla S., Thomas A.M., Nikolayev A.A., Galimova G.R., Azyazov V.N., Mebel A.M., Kaiser R.I. Gas-Phase Synthesis of 3-Vinylcyclopropene via the Crossed Beam Reaction of the Methylidyne Radical ( $\text{CH}$ ;  $X^2\Pi$ ) with 1,3-Butadiene ( $\text{CH}_2\text{CHCHCH}_2$ ;  $X^1A_g$ ) ChemPhysChem, 2020, 21, 1295–1309.
466. Zhao L., Kaiser R.I., Lu W., Ahmed M., Oleinikov A.D., Azyazov V.N., Mebel A.M., Howlader A.H., Wnuk S.F. Gas Phase Formation of Phenalene via  $10\pi$ -Aromatic, Resonantly Stabilized Free Radical Intermediates Phys. Chem. Chem. Phys., 2020, 22, 15381-15388.
467. Singh S.K., Tsai T.-Y., Sun B.-J., Chang A.H.H., Mebel A.M., Kaiser R.I. Gas Phase Identification of the Elusive N-Hydroxyoxaziridine ( $c\text{-H}_2\text{CON}(\text{OH})$ ) – A Chiral Molecule J. Phys. Chem. Lett., 2020, 11, 5383-5389.
468. Doddipatla S., He C., Kaiser R.I., Luo Y., Sun R., Galimova G.R., Mebel A.M., Millar T.J. A Chemical Dynamics Study on the Gas Phase Formation of Thioformaldehyde ( $\text{H}_2\text{CS}$ ) and its Elusive Thiohydroxy-Carbene Isomer ( $\text{HCSH}$ ) Proc. Nat. Acad. Sci., 2020, 117, 22712-22719.
469. Semenikhin A.S., Savchenkova A.S., Chechet I.V., Matveev S.G., Frenklach M., Mebel A.M. On the mechanism of soot nucleation. II. E-bridge formation at PAH bay Phys. Chem. Chem. Phys., 2020, 22, 17196-17204.
470. Yang Z., He C., Doddipatla S., Krasnoukhov V.S., Azyazov V.N., Mebel A.M., Kaiser R.I. Directed Gas Phase Formation of Methylgermylene ( $\text{HGeCH}_3$ ) ChemPhysChem, 2020, 21, 1898-1904.
471. Yang Z., He C., Doddipatla S., Krasnoukhov V.S., Azyazov V.N., Mebel A.M., Kaiser R.I. Directed Gas Phase Formation of Silene ( $\text{H}_2\text{SiCH}_2$ ) Chem. Eur. J., 2020, 26, 13584-13589.

472. Doddipatla S., Yang Z., Thomas A.M., Chen Y.-L., Sun B.J., Chang A.H.H., Mebel A.M., Kaiser R.I.  
Gas Phase Synthesis of the Elusive Trisilacyclopropyl Radical ( $\text{Si}_3\text{H}_5$ ) via Unimolecular Decomposition of Chemically Activated Doublet Trisilapropyl Radicals ( $\text{Si}_3\text{H}_7$ )  
J. Phys. Chem. Lett., 2020, 11, 7874-7881.
473. Tuli L.B., Mebel A.M.  
Formation of Phenanthrene via H-assisted Isomerization of 2-Ethynylbiphenyl Produced in the Reaction of Phenyl with Phenylacetylene  
Int. J. Chem. Kinet., 2020, 52, 875-883.
474. Howlader A.H., Diaz K., Mebel A.M., Kaiser R.I., Wnuk S.F.  
Iodoindenes: Synthesis and application to cross-coupling  
Tetrahedron Letters, 2020, 61, 152427.
475. Zhao L., Kaiser R.I., Lu W., Kostko O., Ahmed M., Evseev M.M., Bashkurov E.K., Oleinikov A.D., Azyazov V.N., Mebel A.M., Howlader A.H., Wnuk S.F.  
Gas Phase Formation of Cyclopentanaphthalene (Benzindene) Isomers via Reactions of 5- and 6-Indenyl Radicals with Vinylacetylene  
Phys. Chem. Chem. Phys., 2020, 22, 22493-22500.
476. Krasnoukhov V.S., Zagidullin M.V., Zavershinskiy I.P., Mebel A.M.  
Formation of Phenanthrene via Recombination of Indenyl and Cyclopentadienyl Radicals: A Theoretical Study  
J. Phys. Chem. A, 2020, 124, 9933-9941.
477. He C., Galimova G.R., Luo Y., Zhao L., Eckhardt A.K., Sun R., Mebel A.M., Kaiser R.I.  
A Chemical Dynamics Study on the Gas Phase Multi Channel Reaction to Triplet Pentadiynylidene ( $\text{HCCCCCH}$ ) and Singlet Ethynylcyclopropenylidene ( $\text{c-C}_5\text{H}_2$ ) Carbenes  
Proc. Nat. Acad. Sci., 2020, 117, 30142-30150.
478. Savchenkova A.S., Chechet I.V., Matveev S.G., Frenklach M., Mebel A.M.  
Formation of phenanthrenyl radicals via the reaction of acenaphthyl with acetylene  
Proc. Combust. Inst., 2021, 38, 1441-1448.
479. Korobeinichev O.P., Trubachev S.A., Joshi A.K., Kumar A., Paletsky A.A., Tereshchenko A.G., Shmakov A.G., Glaznev R.K., Raghavan V., Mebel A.M.  
Experimental and numerical studies of downward flame spread over PMMA with and without addition of triphenyl phosphate  
Proc. Combust. Inst., 2021, 38, 4867-4875.
480. Doddipatla S., Thomas A.M., He C., Yang Z., Kaiser R.I., Galimova G.R., Morozov A.N., Mebel A.M.  
Low Temperature Gas Phase Formation of Indene in the Interstellar Medium  
Science Adv., 2021, 7, eabd4044.
481. Yang Z., Doddipatla S., Kaiser R.I., Krasnoukhov V.S., Azyazov V.N., Mebel A.M.

- Directed Gas Phase Formation of the Elusive Silylgermylidyne Radical ( $\text{H}_3\text{SiGe}, X^2A'$ )  
ChemPhysChem, 2021, 22, 184-191.
482. He C., Nikolayev A.A., Zhao L., Thomas A.M., Doddipatla S., Galimova G.R., Azyazov V.N., Mebel A.M., Kaiser R.I.  
Gas-Phase Synthesis of  $\text{C}_5\text{H}_6$  isomers via the Crossed Beam Reaction of the Methylidyne Radical ( $\text{CH}; X^2\Pi$ ) with 1,2-butadiene ( $\text{CH}_3\text{CHCCH}_2; X^1A'$ )  
J. Phys. Chem. A, 2021, 125, 126-138.
483. Zhao L., Doddipatla S., Kaiser R.I., Lu W., Kostko O., Ahmed M., Tuli L.B., Morozov A.N., Howlader A.H., Wnuk S.F., Mebel A.M., Azyazov V.N., Mohamed R.K., Fischer F.R.  
Gas Phase Synthesis of Corannulene – A Molecular Building Block of Fullerenes – in Circumstellar Envelopes  
Phys. Chem. Chem. Phys., 2021, 23, 5740-5749.
484. Mishra P., Fritz S.M., Herbers S., Mebel A.M., Zwier T.S.  
Gas-phase pyrolysis of trans 3-pentenitrile: competition between direct and isomerization-mediated dissociation  
Phys. Chem. Chem. Phys., 2021, 23, 6462-6471.
485. Yang Z.H., Doddipatla S., Kaiser R.I., Nikolayev A.A., Azyazov V.N., Mebel A.M.  
On the Synthesis of the Astronomically Elusive 1-Ethynyl-3-Silacyclopropenylidene ( $c\text{-SiC}_4\text{H}_2$ ) Molecule in Circumstellar Envelopes of Carbon-rich Asymptotic Giant Branch Stars and Its Potential Role in the Formation of the Silicon Tetracarbide Chain ( $\text{SiC}_4$ )  
Astrophys. J. Lett., 2021, 908, L40.
486. Semenikhin A.S., Savchenkova A.S., Chechet I.V., Matveev S.G., Frenklach M., Mebel A.M.  
Transformation of an Embedded Five-Membered Ring in Polycyclic Aromatic Hydrocarbons via the HACA mechanism: A Theoretical Study  
J. Phys. Chem. A, 2021, 125, 3341-3354.
487. Porfiriev D.P., Azyazov V.N., Mebel A.M.  
Mechanism and Kinetics of the Oxidation of 1,3-Butadien-1-yl ( $n\text{-C}_4\text{H}_5$ ): A Theoretical Study  
Phys. Chem. Chem. Phys., 2021, 23, 9198-9210.
488. Zhao L., Lu W., Ahmed M., Zagidullin M.V., Azyazov V.N., Morozov A.N., Mebel A.M., Kaiser R.I.  
Gas Phase Synthesis of Benzene via the Propargyl Radical Self-Reaction  
Science Adv., 2021, 7, eabf0360.
489. Morozov A.N., Medvedkov Y.A., Azyazov V.N., Mebel A.M.  
Theoretical Study of the Phenoxy Radical Recombination with the  $\text{O}(^3P)$  Atom,  
Phenyl plus Molecular Oxygen Revisited  
J. Phys. Chem. A, 2021, 125, 3965-3977.

490. Krasnoukhov V.S., Azyazov V.N., Mebel A.M., Doddipatla S., Yang Z., Goettl S., Kaiser R.I.  
Combined Crossed Molecular Beams and Ab Initio Study of the Bimolecular Reaction of Ground State Atomic Silicon (Si;  $^3P$ ) with Germane ( $GeH_4$ ;  $X^1A_1$ )  
ChemPhysChem, 2021, 22, 1497-1504.
491. Frenklach M., Semenikhin A.S., Mebel A.M.  
On the Mechanism of Soot Nucleation. III. The Fate and Facility of the E-Bridge  
J. Phys. Chem. A, 2021, 125, 6789-6795.
492. Ghildina A.R., Zavershinskiy I.P., Mebel A.M., Vinogradov K.Yu., Bulanova A.V., Zhu H.  
Theoretical Study of the Mechanism and Kinetics of the Oxidation of Cyclopenta[a]Naphthalenyl Radical  $C_{13}H_9$  with Molecular Oxygen  
J. Phys. Chem. A, 2021, 125, 6796-6804.
493. Yang Z., He C., Goettl S., Kaiser R.I., Azyazov V.N., Mebel A.M.  
Directed Gas-Phase Formation of Aminosilylene ( $HSiNH_2$ ;  $X^1A'$ ) - the Simplest Silicon Analogue of an Aminocarbene - under Single-Collision Conditions  
J. Am. Chem. Soc., 2021, 143, 14227-14234.
494. Zhao L., Prendergast M., Kaiser R.I., Xu B., Lu W., Ahmed M., Howlader A.H., Wnuk S.F., Korotchenko A.S., Evseev M.M., Bashkirov E.K., Azyazov V.N., Mebel A.M.  
A Molecular Beams and Computational Study on the Barrierless Gas Phase Formation of (Iso)Quinoline in Low Temperature Extraterrestrial Environments  
Phys. Chem. Chem. Phys., 2021, 23, 18495-18505.
495. Nikolayev A.A., Azyazov V.N., Kaiser R.I., Mebel A.M.  
Theoretical Study of the Reaction of the Methylidyne Radical ( $CH$ ;  $X^2\Pi$ ) with 1-Butyne ( $CH_3CH_2CCH$ ;  $X^1A'$ )  
J. Phys. Chem. A, 2021, 125, 43, 9536-9547.
496. Pershin A.A., Azyazov V.N., Torbin A.P., Mikheyev P.A., Mebel A.M., Kaiser R.I.  
Ozone Destruction due to the Recombination of Oxygen Atoms  
J. Chem. Phys., 2021, 155, 164307.
497. He C., Doddipatla S., Yang Z., Goettl S.J., Kaiser R.I., Azyazov V.N., Mebel A.M., Millar T.J.  
Gas-Phase Synthesis of Silaformaldehyde ( $H_2SiO$ ) and Hydroxysilylene ( $HSiOH$ ) in Outflows of Oxygen-Rich Asymptotic Giant Branch Stars  
Astrophys. J. Lett., 2021, 921, L7.
498. Monluc L., Nikolayev A.A., Medvedkov I.A., Azyazov V.N., Morozov A.N., Mebel A.M.

The Reaction of o-Benzynes with Vinylacetylene: An Unexplored Way to Produce Naphthalene

ChemPhysChem, 2022, 23, e202100758.

499. Alarcon J.F., Mebel A.M.  
Direct H abstraction by molecular oxygen from unsaturated C3-C5 hydrocarbons: A theoretical study  
Int. J. Chem. Kinet., 2022, 54, 203-217.
500. He C., Fujioka K., Nikolayev A.A., Zhao L., Doddipatla S., Azyazov V.N., Mebel A.M., Sun R., Kaiser R.I.  
A Chemical Dynamics Study of the Reaction of the Methylidyne Radical (CH,  $X^2\Pi$ ) with Dimethylacetylene (CH<sub>3</sub>CCCH<sub>3</sub>,  $X^1A_{1g}$ )  
Phys. Chem. Chem. Phys., 2022, 24, 578-593.
501. Gurusinghe R.M., Dias N., Mebel A.M., Suits A.G.  
Radical–Radical Reaction Dynamics Probed Using Millimeterwave Spectroscopy: Propargyl + NH<sub>2</sub>/ND<sub>2</sub>  
J. Phys. Chem. Lett., 2022, 13, 1, 91–97.
502. Kaiser R.I., Zhao L., Lu W., Ahmed M., Zagidullin M.V., Azyazov V.N., Mebel A.M.  
Gas-Phase Formation of Benzene (C<sub>6</sub>H<sub>6</sub>) and Naphthalene (C<sub>10</sub>H<sub>8</sub>) through Resonantly Stabilized Cyclopentadienyl-Mediated Radical-Radical Reactions  
J. Phys. Chem. Lett., 2022, 13, 1, 208–213.
503. Kaiser R.I., Zhao L., Lu W., Ahmed M., Krasnoukhov V.S., Azyazov V.N., Mebel A.M.  
One Collision – Three Rings: Unconventional Excited-State Dynamics in the Concerted Benzyl (C<sub>7</sub>H<sub>7</sub>) Radical Self-Reaction to Anthracene (C<sub>14</sub>H<sub>10</sub>)  
Nature Commun., 2022, 13, 786.
504. Galimova G.R., Medvedkov I.A., Mebel A.M.  
The Role of Methylaryl Radicals in the Growth of Polycyclic Aromatic Hydrocarbons: The Formation of Five-Membered Rings  
J. Phys. Chem. A, 2022, 126, 1233-1244.
505. Vinogradov K.Yu., Bulanova A.V., Shafigulin R.V., Tokranova E.O., Mebel A.M., Zhu H.  
A density functional theory study of the oxygen reduction reaction mechanism on graphene doped with nitrogen and a transition metal  
ACS Omega, 2022, 7, 7066–7073.
506. Goettl S.J., He C., Paul D., Kaiser R.I., Nikolayev A.A., Azyazov V.N., Mebel A.M.  
Gas-Phase Study of the Elementary Reaction of the D1-Ethynyl Radical (C<sub>2</sub>D;  $X^2\Sigma^+$ ) with Propylene (C<sub>3</sub>H<sub>6</sub>;  $X^1A'$ ) Under Single Collision Conditions  
J. Phys. Chem. A, 2022, 126, 1889–1898.
507. Savchenkova A.S., Semenikhin A.S., Chechet I.V., Matveev S.G., Frenklach M., Morozov A.N., Mebel A.M.

- Mechanism of E-bridge formation by various PAH molecules: A theoretical study  
Chem. Phys. Lett., 2022, 799, 139637.
508. Di S., Liu W., Guo C., Wang F., Bulanova A., Mebel A., Zhu H.  
Hierarchical porous N-doped carbon-supported PtCu nanoparticles as an efficient catalyst for oxygen reduction reaction  
J. Power Sources, 2022, 533, 231270.
509. Torbin A. P., Demyanov A. V., Kochetov I. V., Mikheyev P. A., Mebel A. M.  
Ozone production in a dielectric barrier discharge in air- and oxygen-methane mixtures. Experiment and modeling  
Plasma Sources Sci. Tech., 2022, 31, 035017.
510. Krikunova L.I., Nikolayev A.A., Porfirev D.P., Mebel A.M.  
The reaction of the methylidyne radical ( $\text{CH } X^2\Pi$ ) with the hydrogen cyanide ( $\text{HCN } X^1\Sigma^+$ ) molecule in cold molecular clouds and planetary atmospheres  
J. Biomed. Photon. Eng., 2022, 8, 020301.
511. Zhou C. W., Farooq A., Yang L. J., Mebel A. M.  
Combustion chemistry of alkenes and alkadienes  
Prog. Energy Combust. Sci., 2022, 90, 100983.
512. He C., Goettl S.J., Yang Z., Kaiser R.I., Nikolayev A.A., Azyazov V.N., Mebel A.M.  
Gas-Phase Preparation of Subvalent Germanium Monoxide ( $\text{GeO}, X^1\Sigma^+$ ) via Non-Adiabatic Reaction Dynamics in the Exit Channel  
J. Phys. Chem. Lett., 2022, 13, 4589–4597.
513. Liamtsau V., Liu G., Morozov A.N., Mebel A.M., Cai Y.  
Chromatographic framework for coffee ring effect-driven separation of small molecules in surface enhanced Raman spectroscopy analysis  
Talanta, 2022, 250, 123688.
514. Zhou J., Guo J., Mebel A.M., Ghimire G., Liang F., Chang S., He J.  
Probing the Intermediates of Catalyzed Dehydration Reactions of Primary Amide to Nitrile in Plasmonic Junctions  
ACS Catal., 2022, 12, 7737–7747.
515. Deriu C., Morozov A.N., Mebel A.M.  
Direct and Water-mediated Adsorption of Stabilizers on SERS-active Colloidal Bimetallic Plasmonic Nanomaterials: Insight on Citrate-AuAg Interactions from DFT Calculations  
J. Phys. Chem. A, 2022, 126, 32, 5236–5251.
516. Cui D., Abdullah A.M., Peller J. R., Mezyk S.P., Mebel A., O'Shea K.  
Effectiveness of Photocatalysis, Radiolysis, and Ultrasonic Irradiation in the Remediation of GenX: Computational Study of the Ultrasonically Induced Mineralization  
J. Environ. Eng., 2022, 148, 04022073.
517. Galimova G.R., Mebel A.M., Goettl S.J., Yang Z., Kaiser R.I.

- A Crossed Molecular Beams and Computational Study on the Unusual Reactivity of Banana Bonds of Cyclopropane ( $c\text{-C}_3\text{H}_6$ ;  $X^1A_1'$ ) through Insertion by Ground State Carbon Atoms ( $C(^3P_j)$ )  
 Phys. Chem. Chem. Phys., 2022, 24, 22453-22463.
518. Mebel A.M., Frenklach M.  
 Cleavage of an aromatic ring and radical migration  
 Faraday Discuss., 2022, 238, 512–528.
519. Kaiser R.I., Zhao L., Lu W., Ahmed M., Evseev M.M., Azyazov V.N., Mebel A.M., Mohamed R.K., Fischer F.R.  
 Gas-Phase Synthesis of Racemic Helicenes and their Potential Role in the Enantiomeric Enrichment of Sugars and Aminoacids in Meteorites  
 Phys. Chem. Chem. Phys., 2022, 24, 25077-25087.
520. He, C., Yang, Z., Doddipatla S., Thomas A.M., Kaiser R.I., Galimova G.R., Mebel A.M., Fujioka K., Sun R.  
 Directed Gas Phase Preparation of Ethynylallene ( $\text{CH}_2\text{CCHCCH}$ ;  $X^1A_1'$ ) via the Crossed Molecular Beam Reaction of the Methylidyne Radical ( $\text{CH}$ ;  $X^2\Pi$ ) with Vinylacetylene ( $\text{H}_2\text{CCHCCH}$ ;  $X^1A_1'$ )  
 Phys. Chem. Chem. Phys., 2022, 24, 26499-26510.
521. Rue K. L., Mathivathanan L., Mezei G., Mebel A.M., Raptis R.G.  
 Crystal Structure, Hirshfeld Analysis, and DFT Calculations of Three Trinuclear Cu(II) Polymorphs  
 Crystals 2022, 12, 1611.
522. Yang Z., Galimova G.R., He C., Doddipatla S., Mebel A.M., Kaiser R.I.  
 Gas Phase Preparation of 1,3,5,7-Cyclooctatetraene ( $\text{C}_8\text{H}_8$ ) through Ring Expansion via the Aromatic 1,3,5-Cyclooctatrien-7-yl Radical ( $\text{C}_8\text{H}_9^\bullet$ )  
 Transient  
 J. Am. Chem. Soc., 2022, 144, 22470-22478.
523. Paultre C.B., Mebel A.M., O'Shea K.E.  
 Computational study of the gas-phase thermal degradation of perfluoroalkyl carboxylic acids  
 J. Phys. Chem. A, 2022, 126, 8753-8760.
524. Frenklach M., Mebel A.M.  
 On the Mechanism of Soot Nucleation. IV. Molecular Growth of the Flatten E-Bridge  
 J. Phys. Chem. A, 2022, 126, 9259-9267.

525. Morozov A.N., Mebel A.M., Frenklach M.  
Acceleration of a Chemical Reaction due to Non-Equilibrium Collisional Dynamics: Dimerization of Polyaromatics  
J. Phys. Chem. Lett., 2022, 13, 11528-11535.
526. Wang J., Marks J.H., Tuli L.B., Mebel A.M., Azyazov V.N., Kaiser R.I.  
The Formation of Thioformic Acid (HCOSH) – the Simplest Thioacid – in Interstellar Ice Analogs  
J. Phys. Chem. A, 2022, 126, 9699-9708.
527. Krasnoukhov V.S., Pivovarov P.S., Zagidullin M.V., Azyazov V.N., Mebel A.M., Morozov A.N.  
Formation of Two-ring Polycyclic Aromatic Hydrocarbons via the Recombination of Benzyl and Propargyl Radicals under the Circumstellar Envelopes Conditions of Asymptotic Giant Branch Stars  
Astron. Rep., 2022, 66, 811-826.
528. Wang J., Marks J.H., Turner A.M., Nikolayev A.A., Azyazov V.N., Mebel A.M., Kaiser R.I.  
Mechanistical study on the formation of hydroxyacetone ( $\text{CH}_3\text{COCH}_2\text{OH}$ ), methyl acetate ( $\text{CH}_3\text{COOCH}_3$ ), and 3-hydroxypropanal ( $\text{HCOCH}_2\text{CH}_2\text{OH}$ ) along with their enol tautomers (prop-1-ene-1,2-diol ( $\text{CH}_3\text{C}(\text{OH})\text{CHOH}$ ), prop-2-ene-1,2-diol ( $\text{CH}_2\text{C}(\text{OH})\text{CH}_2\text{OH}$ ), 1-methoxyethen-1-ol ( $\text{CH}_3\text{OC}(\text{OH})\text{CH}_2$ ) and prop-1-ene-1,3-diol ( $\text{HOCH}_2\text{CHCHOH}$ )) in interstellar ice analogs  
Phys. Chem. Chem. Phys., 2023, 25, 936-953.
529. Alarcon J.F., Ajo S., Morozov A.N., Mebel A.M.  
Theoretical study on the mechanism and kinetics of the oxidation of allyl radical with atomic and molecular oxygen  
Combust. Flame, 2023, 249, 112388.
530. Frenklach M., Mebel A. M.  
Prenucleation chemistry of aromatics: A two-ring precursor?  
Proc. Combust. Inst., 2023, 39, 825–833.
531. Tuli L.B., Mebel A. M., Frenklach M.  
Bay capping via acetylene addition to polycyclic aromatic hydrocarbons: Mechanism and kinetics  
Proc. Combust. Inst., 2023, 39, 969–977.
532. Krikunova L.I., Nikolayev A.A., Porfiriev D.P., Mebel A.M.  
Reaction of Propionitrile with Methylidyne: A Theoretical Study  
J. Chin. Chem. Soc., 2023, 70, 439–450.
533. Shmakov A.G., Korobeinichev O.P., Mebel A.M., Porfiriev D.P., Ghildina A.R., Osipova K.N., Knyazkov D.A., Gerasimov I.E., Liu Z., Yang B.  
High-Temperature Thermal Decomposition of Triphenyl Phosphate Vapor in an Inert Medium: A Flow Reactor Pyrolysis, Quantum Chemical Calculations and Kinetic Modeling  
Combust. Flame, 2023, 249, 112614.

534. He C., Kaiser R.I., Lu W., Ahmed M., Pivovarov P.S., Kuznetsov O.V., Zagidullin M.V., Mebel A.M.  
Unconventional Dynamics in the Gas-Phase Synthesis of 9H-Fluorene (C<sub>13</sub>H<sub>10</sub>) via the Benzyl – Phenyl Radical – Radical Reaction  
Angew. Chem., Int. Ed., 2023, 62, e202216972.
535. He C., Kaiser R.I., Lu W., Ahmed M., Reyes Y., Wnuk S.F. Mebel A.M.  
Exotic Reaction Dynamics in the Gas Phase Preparation of Anthracene (C<sub>14</sub>H<sub>10</sub>) via Spiroaromatic Radical Transients in the Indenyl – Cyclopentadienyl Radical – Radical Reaction  
J. Am. Chem. Soc., 2023, 145, 3084-3091.
536. Tuli, L.B., Goettl S.J., Turner, A.M., Howlader A.H., Hemberger P., Wnuk S.F., Guo T., Mebel A.M., Kaiser R.I.  
Gas Phase Synthesis of the C<sub>40</sub> Nano Bowl (C<sub>40</sub>H<sub>10</sub>)  
Nature Commun., 2023, 14, 1527.
537. Wang J., Marks J.H., Turner A.M., Mebel A.M., Eckhardt A.K., Kaiser R.I.  
Gas Phase Detection of Oxirene  
Science Adv., 2023, 9, eadg1134.
538. Selby T.M., Goulay F., Soorkia S., Ray A., Jasper A.W., Klippenstein S.J., Morozov A.N., Mebel A.M., Savee J.D., Taatjes C.A., Osborn D.L.  
Radical-Radical Reactions in Molecular Weight Growth: The Phenyl + Propargyl Reaction  
J. Phys. Chem. A, 2023, 127, 2577–2590.
539. Mebel A.M., Agúndez M., Cernicharo J., Kaiser R.I.  
Elucidating the Formation of Ethynylbutatrienylidene (HCCCHCCC; X<sup>1</sup>A') in the Taurus Molecular Cloud (TMC-1) via the Gas Phase Reaction of Tricarbon (C<sub>3</sub>) with the Propargyl Radical (C<sub>3</sub>H<sub>3</sub>)  
Astrophys. J. Lett., 2023, 945, L40 (8 pp.).
540. Mejia G., Su L., Pandey P., Jeanne Dit Fouque K., McGoron A., Fernandez-Lima F., He J., Mebel A.M., Leng F.  
Anticancer drug doxorubicin spontaneously reacts with GTP and dGTP  
Chem. Research Tox., 2023, 36, 660–668.
541. He C., Kaiser R.I., Lu W., Ahmed M., Krasnoukhov V.S., Pivovarov P.S., Zagidullin M.V., Azyazov V.N., Morozov A.N., Mebel A.M.  
Unconventional Gas-Phase Preparation of the Prototype Polycyclic Aromatic Hydrocarbon Naphthalene (C<sub>10</sub>H<sub>8</sub>) via the Reaction of Benzyl (C<sub>7</sub>H<sub>7</sub>) and Propargyl (C<sub>3</sub>H<sub>3</sub>) Radicals Coupled with Hydrogen-Atom Assisted Isomerization  
Chem. Sci., 2023, 14, 5369-5378.

542. Wang J., Nikolayev A.A., Marks J.H., Mcanally M., Azyazov V.N., Eckhardt A.K., Mebel A.M., Kaiser R.I.  
Quantum Tunneling Mediated Low-Temperature Synthesis of Interstellar Hemiacetals - Key Intermediates for a Prebiotic Sugar Formation  
J. Phys. Chem. Lett., 2023, 14, 6078–6085.
543. Wang J., Nikolayev A.A., Zhang C., Marks J.H., Azyazov V.N., Eckhardt A.K., Mebel A.M., Kaiser R.I.  
Synthesis of interstellar propen-2-ol ( $\text{CH}_3\text{C}(\text{OH})\text{CH}_2$ ) – the simplest enol tautomer of a ketone  
Phys. Chem. Chem. Phys., 2023, 25, 17460-17469.
544. Goettl S.J., Yang Z., Kollotzek S., Paul D., Kaiser R.I., Somani A., Portela-González A., Sander W., Nikolayev A.A., Azyazov V.N., Mebel A.M.  
Exploring the Chemical Dynamics of Phenylethynyl Radical ( $\text{C}_6\text{H}_5\text{CC}$ ;  $\text{X}^2\text{A}_1$ ) Reactions with Allene ( $\text{H}_2\text{CCCH}_2$ ;  $\text{X}^1\text{A}_1$ ) and Methylacetylene ( $\text{CH}_3\text{CCH}$ ;  $\text{X}^1\text{A}_1$ )  
J. Phys. Chem. A., 2023, 127, 5723–5733.
545. Goettl S.J., Tuli L.B., Turner A.M., Reyes Y., Howlader A.H., Wnuk S.F., Hemberger P., Mebel A.M., Kaiser R.I.  
Gas Phase Synthesis of Coronene through a Directed Ring Annulation Framework  
J. Am. Chem. Soc., 2023, 145, 15443–15455.
546. Rue K.L., Herrera S., Chakraborty I., Mebel A.M., Raptis R.G.  
Completion of Crystallographic Data for the Series of 4-Halogenated-1*H*-pyrazoles: Crystal Structure Determination of 4-Iodo-1*H*-pyrazole and Spectroscopic Comparison  
Crystals 2023, 13, 1101 (12 pp.).
547. Marks J.H., Nikolayev A.A., Evseev M.M., Wang J., Turner A.M., Kleimeier N. F., Kuznetsov O.V., McAnally M., Morozov A.N., Antonov I.O., Mebel A.M., Kaiser R.I.  
Quantum Tunneling Mediated Synthesis of Prebiotic Chelation Agents in Interstellar Analog Ices  
CHEM, 2023, 9, 3286-3303.
548. Yang Z., Galimova G.R., He C., Goettl S., Paul D., Lu W., Ahmed M., Mebel A.M., Li Xi., Kaiser R.I.  
Gas-Phase Formation of the Resonantly Stabilized 1-Indenyl ( $\text{C}_9\text{H}_7^\cdot$ ) Radical in the Interstellar Medium  
Science Adv., 2023, 9, eadi5060.
549. Li W., Yang J., Zhao L., Couch D., San Marchi M., Hansen N., Morozov A.N., Mebel A.M., Kaiser R.I.  
Unexpected Gas-Phase Preparation of Azulene ( $\text{C}_{10}\text{H}_8$ ) via Reaction of the Resonantly Stabilized Fulvenallenyl ( $\text{C}_7\text{H}_5^\cdot$ ) and Propargyl ( $\text{C}_3\text{H}_3^\cdot$ ) Radicals  
Chem. Sci., 2023, 14, 9795-9805.

550. Zhou J., Guo J., Ghimire G., Mebel A.M., Chang S., He J.  
Plasmon-mediated dehydrogenation of the aromatic methyl group and benzyl radical formation  
Chem. Sci, 2023, 14, 13951-13961.
551. Medvedkov I.A., Nikolayev A.A., He C., Yang Z., Mebel A.M., Kaiser R.I.  
A Combined Experimental and Computational Study on the Reaction Dynamics of the 1-Propynyl ( $\text{CH}_3\text{CC}$ ,  $X^2A_1$ ) – Propylene ( $\text{CH}_3\text{CHCH}_2$ ,  $X^1A'$ ) System: Formation of 1,3-Dimethylvinylacetylene ( $\text{CH}_3\text{CCCHCHCH}_3$ ,  $X^1A'$ ) under Single Collision Conditions  
Mol. Phys., 2024, 122, e2234509.
552. Medvedkov I.A., Nikolayev A.A., He C., Yang Z., Mebel A.M., Kaiser R.I.  
One Collision – Two Substituents: Gas-Phase Preparation of Xylenes under Single-Collision Conditions  
Angew. Chem., Int. Ed., 2024, 63, e202315147.
553. Paultre C.-B., Mebel A.M., O'Shea K.E.  
Reaction Rate Coefficient Study of the Perfluoroalkyl and  $\omega$ -Perfluoroalkyloic Acid Radicals  
Chem. Phys. Lett., 2024, 838, 141077.
554. Medvedkov I.A., Nikolayev A.A., Yang Z., Goettl S.J., Mebel A.M., Kaiser R.I.  
Elucidating the Chemical Dynamics of the Elementary Reactions of the 1-Propynyl Radical ( $\text{CH}_3\text{CC}$ ;  $X^2A_1$ ) with 2-Methylpropene ( $(\text{CH}_3)_2\text{CCH}_2$ ;  $X^1A_1$ )  
Phys. Chem. Chem. Phys., 2024, 26, 6448-6457.
555. Reyes Y., Mebel A., Wnuk S.F.  
6-azido and 6-azidomethyl uracil nucleosides  
Nucleos. Nucleot. Nucl., 2024, 43, 453-471.
556. Fang, Y., Liu, G., Wang, Y., Yin, Y., Cai, Y., Mebel, A.M., Jiang, G.  
Transformation of Mercurous [Hg(II)] Species During Laboratory Standard Preparation and Analysis: Implication for Environmental Analysis  
Environ. Sci. Tech., 2024, 58, 6825-6834.
557. Frenklach M., Jasper A.W., Mebel A.M.  
Phenalenyl Growth Reactions and Implications to Prenucleation Chemistry of Aromatics in Flames  
Phys. Chem. Chem. Phys., 2024, 26, 13034-13048.
558. Marks J.H., Bai X., Nikolayev A.A., Gong Q., Zhu C., Kleimeier N.F., Turner A.M., Singh S.K., Wang J., Yang J., Pan Y., Yang T., Mebel A.M., Kaiser R.I.  
Methanetriol — Formation of an Impossible Molecule  
J. Am. Chem. Soc., 2024, 146, 12174-12184.
559. Yang Z., He C., Goettl S.J., Mebel A.M., Velloso P.F.G., Alves M.O., Galvão B.R. L., Kaiser R.I.

- Low-Temperature Gas-Phase Synthesis of Methylene Amidogen ( $\text{H}_2\text{CN}$ ) and Cyanomethyl ( $\text{H}_2\text{CCN}$ ) Radicals and their Role in the Formation of Pyridine and (Iso)quinoline in Hydrocarbon-Rich Atmospheres of Planets and their Moons  
*Nature Astron.*, 2024, 8, 856–864.
560. Goettl S.J., Yang Z., He C., Somani A., Portela-Gonzalez A., Sander W., Mebel A.M., Kaiser R.I.  
Exploring the Chemical Dynamics of Phenanthrene ( $\text{C}_{14}\text{H}_{10}$ ) Formation via the Bimolecular Gas-Phase Reaction of the Phenylethynyl Radical ( $\text{C}_6\text{H}_5\text{CC}$ ) with Benzene ( $\text{C}_6\text{H}_6$ )  
*Faraday Discuss.*, 2024, 251, 509-522.
561. Erkok S.D., Hernandez E., Cruz J., Mebel A.M., McCord B.  
Differentiating Structurally Similar Fentanyl Analogs by Comparing Density Functional Theory (DFT) Calculations and Surface-Enhanced Raman Spectroscopy (SERS) Results  
*Appl. Spectrosc.*, 2024, 78, 667-679.
562. Shmakov A.G., Gerasimov I.E., Knyazkov D.A., Osipova K.N., Korobeinichev O.P., Trubachev S.A., Mebel A.M., Porfiriev D.P., Ghildina A.R.  
Development of the Detailed Mechanism of Pyrolysis and Combustion of Triphenyl Phosphate: New Quantum Chemistry Calculations and Experimental Data on Structure of the  $\text{H}_2/\text{O}_2/\text{Ar}$  Flame Doped with TPP  
*Combust. Flame*, 2024, 266, 113534.
563. Mebel A.M., Li W., Pratali Maffei L., Cavallotti C., Morozov A.N., Wang C.-Y., Yang J.-Z., Zhao L., Kaiser R.I.  
Fulvenallenyl Radical ( $\text{C}_7\text{H}_5^*$ ) Mediated Gas-Phase Synthesis of Bicyclic Aromatic  $\text{C}_{10}\text{H}_8$  Isomers: Can Fulvenallenyl Efficiently React with Closed-Shell Hydrocarbons?  
*J. Phys. Chem. A*, 2024, 128, 5707–5720.
564. Alarcon J.F., Morozov A.N., Mebel A.M., Della Libera A., Pratali Maffei L., Cavallotti C.  
Mechanism and Kinetics of the Oxidation of Propargyl Radical by Atomic Oxygen  
*Proc. Combust. Inst.*, 2024, 40, 105372.
565. Jin H., Mebel A.M., Farooq A.  
Acetylene Addition to the Fulvenallenyl Moiety in Aromatic Hydrocarbons  
*Proc. Combust. Inst.*, 2024, 40, 105777.
566. Miller S.A., Jeanne Dit Fouque K., Mebel A.M., Brown Chandler K., Fernandez-Lima F.  
Gas-Phase Structures of Fucosylated Oligosaccharides: Alkali Metal and Halogen Influences  
*J. Phys. Chem. A*, 2024, 128, 8869–8877.

567. Savchenkova A.S., Chechet I.V., Matveev S.G., Konnov A.A., Mebel A.M.  
Reaction Mechanism of Pyridine Radicals with Molecular Oxygen: A  
Theoretical Study  
Comput. Theor. Chem., 2024, 1241, 114883.
568. Wang J., Nikolayev A.A., Marks J.H., Turner A.M., Chandra S., Kleimeier N.  
F., Young L.A., Mebel A.M., Kaiser R.I.  
Interstellar Formation of Nitrogen Heteroaromatics [Indole, C<sub>8</sub>H<sub>7</sub>N; Pyrrole,  
C<sub>4</sub>H<sub>5</sub>N; Aniline, C<sub>6</sub>H<sub>5</sub>NH<sub>2</sub>] – Precursors to Amino Acids and Nucleobases  
J. Am. Chem. Soc., 2024, 146, 41, 28437–28447.
569. Medvedkov I.A., Nikolayev A.A., Goettl S., Yang Z., Mebel A.M., Kaiser R.I.  
Experimental and Theoretical Study of the Sn – O Bond Formation between  
Atomic Tin and Molecular Oxygen  
Phys. Chem. Chem. Phys., 2024, 26, 27763-27771.
570. Yang Z., Medvedkov I.A., Goettl S.J., Nikolayev A.A., Mebel A.M., Li X.,  
Kaiser R.I.  
Low-Temperature Gas-Phase Formation of Cyclopentadiene in the Interstellar  
Medium  
Proc. Nat. Acad. Sci., 2024, 121, e2409933121.
571. Morozov A.N., Mebel A.M., Frenklach M.  
Monomer Size Effect in Inelastic Collisional Dynamics of Non-Equilibrium  
Soot Nucleation  
J. Chem. Phys., 2024, 161, 234301.
572. Nikolayev A.A., Evseev M.M., Krasnoukhov V.S., Kuznetsova A.A., Pivovarov  
P.P., Porfiriev D.P., Mebel A.M., Kaiser R.I.  
Functionalization of Pyrimidine and Purine to RNA Bases in Water/Ammonia  
Ices via Radical Substitution Reactions  
New. J. Chem., 2025, 49, 332–344.
573. Medvedkov I.A., Yang Z., Nikolayev A.A., Goettl S., Eckhardt A.K., Mebel  
A.M., Kaiser R.I.  
Binding the Power of Cycloaddition and Cross-Coupling in a Single  
Mechanism: An Unexpected Bending Journey to Radical Chemistry of  
Butadiynyl with Conjugated Dienes  
J. Phys. Chem. Lett., 2025, 16, 658–666.
574. Yang Z., Fujioka K., Galimova G.R., Medvedkov I.A., Goettl S.J., Sun R., Li  
X., Mebel A.M., Kaiser R.I.  
Directed Gas-Phase Formation of Azulene (C<sub>10</sub>H<sub>8</sub>): Unraveling the Bottom-Up  
Chemistry of Saddle-Shaped Aromatics  
ACS Central Sci., 2025, 11, 322-330.
575. Paultre C.-B., Mebel A.M., O'Shea K.E.  
Computational Study of the Gas-Phase Thermal Degradation and the  
Reaction Rate Coefficients of Perfluoroalkyl Ether Carboxylic Acids  
J. Phys. Chem. A, 2025, 129, 1856-1868.

576. Medvedkov I.A., Nikolayev A.A., Yang Z., Goettl S.J., Kuznetsova A.A., Eckhardt A.K., Mebel A.M., Kaiser R.I.  
A Combined Crossed Molecular Beam and Theoretical Investigation of the Elementary Reaction of Tricarbon ( $C_3(X^1\Sigma_g^+)$ ) with Diacetylene ( $C_4H_2(X^1\Sigma_g^+)$ ): Gas Phase Formation of the Heptatriynylidyne Radical ( $I-C_7H(X_2\Pi)$ )  
J. Phys. Chem. A, 2025, 129, 17, 3931–3939.
577. Goettl S.J., Turner A.M., Krasnoukhov V.S., Azyazov V.N., Kanayama K., Hemberger P., Mebel A.M., Kaiser R.I.  
Gas-Phase Synthesis of Anthracene and Phenanthrene via Counterintuitive Radical–Radical Reaction Induced Ring Expansions  
Science Adv., 2025, 11, eadv0692.
578. Morozov A.N., Pratali Maffei L., Mebel A.M.  
Rate Constants of the Fulvenallenyl Recombination with Propargyl and Its Role in PAH Formation: A Theoretical and Kinetic Modeling Study  
Phys. Chem. Chem. Phys., 2025, 27, 11577–11596.
579. Krivovicheva V., Gangireddy M.S.R., Liu A., Maya L.B., Mebel A.M., Bukhryakov K.V.  
Vanadium-Mediated Carbon Isotope Exchange of Terminal Alkenes  
J. Am. Chem. Soc., 2025, 147, 24, 20212–20217.
580. Marks J., Bai X., Nikolayev A.A., Gong Q., McAnally M., Wang J., Pan Y., Fortenberry R., Mebel A.M., Yang T., Kaiser R.I.  
Methanetetrol and the Final Frontier in Ortho Acids  
Nature Commun., 2025, 16, 6468.
581. Goettl S.J., Ahmed M., Mebel A.M., Kaiser R.I.  
Molecular Mass Growth Processes to Polycyclic Aromatic Hydrocarbons through Radical–Radical Reactions Exploiting Photoionization Reflectron Time-of-Flight Mass Spectrometry  
Acc. Chem. Res., 2025, 58, 2682-2694.
582. Kuznetsov O.V., Evseev M.M., Medvedkov I.A., Tolstov G.I., Khvatov N.A., Antonov I.O., Kaiser R.I., Mebel A.M., Azyazov V.N.  
Products of the Phenyl Radical ( $C_6H_5, X^2A_1$ ) - Acetylene ( $C_2H_2, X^1\Sigma_g^+$ ) Reaction in the 800-1,200 K Temperature Range  
Chem. Eur. J., 2025, e02477 (11 pp.).
583. Medvedkov I.A., Nikolayev A.A., Goettl S.J., Yang Z., Mebel A.M., Kaiser R.I.  
From the Laboratory to Space: Unveiling Isomeric Diversity of  $C_5H_2$  in the Reaction of Tricarbon ( $C_3, X^1\Sigma_g^+$ ) with the Vinyl Radical ( $C_2H_3, X^2A'$ )  
Chem. Sci., 2025, 16, 17859-17866.
584. Mebel A.M., Frenklach M.  
Edge Migration of Aromatic Rings—Kinetics and Directionality  
J. Phys. Chem. A, 2025, 129, 10647-10654.
585. Goettl S.J., Medvedkov I., Nikolayev A., He C., Yang Z., Mebel A.M., Somani A., Portela-Gonzalez A., Sander W., Kaiser R.I.

- Gas-phase synthesis of naphthalene through an unconventional thermal alkyne–alkene [2 + 2] cycloaddition mechanism  
Chem. Sci., 2025,16, 22621-22629.
586. Yang Z., Galimova G.R., He C., Goettl S.J., Mebel A.M., Kaiser R.I.  
An Unconventional Dark Radical Chemistry in Dense Molecular Cloud:  
Directed Gas-Phase Formation of Naphthyl Radicals  
J. Am. Chem. Soc., 2025, 147, 47359–47369.
587. Konnov A.A., Savchenkova A.S., Xie J., Matveev S.S., Matveev S.G., Mebel A.M.  
Theoretical Kinetic Study of the Reactions between Pyridyl Radicals and O<sub>2</sub>  
Fuel, 2026, 405, 136713 (9 pp.).
588. Xie J., Savchenkova A.S., Mebel A.M., Konnov A.A.  
Revisiting the kinetics of pyridine pyrolysis. Part 1: H atom abstraction  
reactions  
Comput. Theor. Chem., 2026, 1255, 115555 (7 pp.).
589. Goettl S.J., Hartwig A., Yang Z., Mebel A.M., Kaiser R.I.  
Directed Gas-Phase Formation of the 1-Cyanovinyl Radical (H<sub>2</sub>CCCN, X<sup>2</sup>A')  
in the Interstellar Medium  
J. Phys. Chem. A, 2026, 130, 242–249.
590. Medvedkov I.A., Nikolayev A.A., Mebel A.M., Yang Z., Goettl S.J., Kaiser R.I.  
The Hidden Path to the Resonance-Stabilized Fulvenallenyl Radical (C<sub>7</sub>H<sub>5</sub>)  
via the Bimolecular Reaction of Tricarbon (C<sub>3</sub>, X<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) with 1,3-Butadiene  
(C<sub>4</sub>H<sub>6</sub>; X<sup>1</sup>A<sub>g</sub>)  
J. Phys. Chem. Lett., in press.
591. Marks J.H., Nikolayev A.A., Wang J., Antonov I.O., Mebel A.M., Kaiser R.I.  
Astrochemistry Prefers the Biomolecule: Isomer-Selective Production of  
Ethanolamine (HOCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>) in Interstellar Model Ices  
Phys. Chem. Chem. Phys., in press.
592. Biswas S., Goettl S.J., Krasnoukhov V.S., Dias N., Azyazov V.N., Arias S.,  
Wnuk S.F., Ahmed M., Mebel A.M., Kaiser R.I.  
Circumstellar Origin of Chrysene (C<sub>18</sub>H<sub>12</sub>) via Self-Recombination of  
Resonantly-Stabilized 1-Indenyl Radicals and Implication to the Aromaticity of  
the Carbonaceous Asteroid Ryugu  
Angew. Chem., Int. Ed., submitted.
593. Zhang C., Leyva V., Nikolayev A.A., Wang J., Turner A.M., Mcanally M.,  
Herath A., Young L.A., Meinert C., Mebel A.M., Kaiser R.I.  
Ammonia-Catalyzed Sugar Formation in the Kuiper Belt  
Nature Comm., submitted.

## Books, Book Chapters, and Conference Proceedings

1. Mebel A.M., Charkin O.P., Solntsev K.A., Kuznetsov N.T.  
Theoretical investigation of structure and structural non-hardness of boron hydride  $B_nH_{n+1}^-$  ( $n = 6-12$ ).  
In: "Chemistry of nonorganic hydrides". Moscow : Nauka, 1990, 43-66.
2. Hsu C.-C., Boughton J.W., Mebel A.M., Lin M.C.  
Theoretical study of HONO reactions with H, OH, NO and  $NH_2$  radicals.  
In "Challenges in Propellants and Combustion. 100 Years after Nobel," Kuo K. K., Ed., Begell House: New York, 1997, pp. 48-57.
3. Mebel A.M., Hayashi M., Lin S.H.  
Ab Initio calculations of spectroscopy and dynamics of polyatomic molecules in Research Trends in Physical Chemistry (Research Trends, India, 1997), vol. 6, pp. 315-341.
4. Mebel A.M., Moskaleva L.V., Lin M.C.  
Reactions of  $NH_2$  in the gas phase.  
In "The chemistry of the N-centered radicals," Alfassi Z.B., editor, Wiley, Chichester, UK, 1998, pp. 467-514.
5. Mebel A.M.  
Dissociation, izomerization, and isotope scrambling of benzene: A theoretical view  
In Reviews of Modern Quantum Chemistry. A Celebration of the Contributions of Robert G. Parr, edited by K. D. Sen  
World Scientific, Singapore, 2002, pp. 340-358.
6. Liang K.K., Jiang J.C., Kislov V.V., Mebel A.M., Lin S.H.  
The Crude Born-Oppenheimer Adiabatic Approximation of Molecular Potential Energies  
In Advances in Chemical Physics, Volume 124, The Role of Degenerate States in Chemistry, edited by M. Baer and G.D. Billing  
Wiley, New York, 2002, pp. 505-555.
7. Mebel A.M.  
Ab initio potential energy surfaces of large reaction systems  
In Modern Trends in Chemical Reaction Dynamics, edited by X. Yang and K. Liu, Advanced Series in Physical Chemistry, vol. 14  
World Scientific, Singapore, 2004, pp. 145-208.
8. Kaiser R.I., Bernath P., Osamura Y., Petrie S., Mebel A.M., Editors.  
Astrochemistry. (Proceedings From Laboratory Studies to Astronomical Observations held in Honolulu, Hawaii 18-20 December 2005.)  
[In: AIP Conf. Proc., 2006; 855], 2006, 324 pp.
9. Jamieson C.S., Mebel A.M., Kaiser R.I.  
  
Investigating the formation of intermediates in the reactions of carbon dioxide ( $CO_2$ ) with suprathermal oxygen and nitrogen atoms.

- AIP Conference Proceedings, 2006, 855 (Astrochemistry), 100-106.
10. Guo Y., Gu X., Zhang F., Mebel A.M., Kaiser R.I.  
Reaction dynamics of small carbon clusters with unsaturated hydrocarbons in the interstellar medium.  
AIP Conference Proceedings, 2006, 855 (Astrochemistry), 42-52.
  11. Mebel A.M., Zyubin A.S., Hayashi M., Lin S.H.  
Ab initio calculations of electronic transitions and photoabsorption and photoluminescence spectra of silica and germania nanoparticles  
In Thin Films and Nanostructures. Physico-Chemical Phenomena in Thin Films and at Solid Surfaces, Vol. 34. Edited by L. I. Trakhtenberg, S. H. Lin and O. J. Ilegbusi. Elsevier, Amsterdam, 2007. pp. 67-120.
  12. Lin S.H., Liang K.K., Hayashi M., Mebel A.M.  
Density matrix treatments of ultrafast radiationless transitions  
In Thin Films and Nanostructures. Physico-Chemical Phenomena in Thin Films and at Solid Surfaces, Vol. 34. Edited by L. I. Trakhtenberg, S. H. Lin and O. J. Ilegbusi. Elsevier, Amsterdam, 2007. pp. 121-182.
  13. Hayashi M., Mebel A.M., Lin S.H.  
Ultrafast radiationless transitions  
In Thin Films and Nanostructures. Physico-Chemical Phenomena in Thin Films and at Solid Surfaces, Vol. 34. Edited by L. I. Trakhtenberg, S. H. Lin and O. J. Ilegbusi. Elsevier, Amsterdam, 2007. pp. 183-227.
  14. Mebel A.M., Kislov V.V., Kaiser R.I.  
Theoretical studies of potential energy surfaces and product branching ratios for the reactions of C<sub>2</sub> with small unsaturated hydrocarbons (acetylene, ethylene, methylacetylene, and allene)  
In Gas Phase Molecular Reactions and Photodissociation Dynamics, edited by K. C. Lin and P. D. Kleiber; Transworld Research Network, Kerala, India, 2007, pp. 113-159.
  15. Pershin A.A., Mebel A.M., Zagidullin M.V., Insapov A.S., Azyazov V.N.  
Ab initio Calculations of Transition Dipole Moments of (O<sub>2</sub>)<sub>2</sub> Complex  
International Conference Laser Optics (LO), St Petersburg, Russia, Jun. 27-Jul. 01, 2016.
  16. Tolstov G.I., Naumkin S.N., Torbin A.P., Mebel A.M., Heaven M.C., Azyazov V.N.  
Products of reaction Rb with C<sub>2</sub>H<sub>6</sub> or CH<sub>4</sub>  
International Conference Laser Optics (LO), St Petersburg, Russia, Jun. 27-Jul. 01, 2016.
  17. Azyazov V.N., Torbin A.P., Mebel A.M., Bresler S., Heaven M.C.

Deactivation and reactions of excited states of Rb in collisions with CH<sub>4</sub> and C<sub>2</sub>H<sub>6</sub>, High Energy/Average Power Lasers and Intense Beam Applications IX, Proceedings of SPIE, Davis S.J., Heaven M.C., Schriempf J.T., Eds., v. 9729, Article # 972909, DOI: 10.1117/12.2218119, SPIE-INT Soc. Optical Engineering, Bellingham, WA, USA  
San Francisco, CA, Feb. 15-16, 2016.

18. Lockhart J., Lynch P.T., Annesley C.J., Mebel A.M., Klippenstein S.J., Tranter R.S.  
A shock tube laser schlieren study of phenyl chloride pyrolysis  
US Combustion Meeting, 10th, College Park, MD, United States, Apr. 23-24, (2017), 2, 1327-1332.
19. Tolstov G.I., Zagidullin M.V., Khvatov N.A., Medvedkov I.A., Mebel, A.M., Heaven M.C., Azyazov V.N.  
Measurements of rate constants of O<sub>2</sub>(b) quenching by CH<sub>4</sub>, NO, N<sub>2</sub>O at temperatures 300-800 K  
MATEC Web of Conferences (2018), 209, 00006/1-00006/5.
20. Galimova G., Azyazov V., Mebel A.  
Quantum chemical study of the mechanism of oxidation of C<sub>15</sub>H<sub>9</sub> by atomic oxygen  
MATEC Web of Conferences (2018), 209, 00008/1-00008/4.
21. Torbin A., Pershin A., Zagidullin M., Heaven M., Mebel A., Azyazov V.  
Ozone recovery in the presence of CO and N<sub>2</sub>O  
MATEC Web of Conferences (2018), 209, 00016/1-00016/6.
22. Azyazov V.N., Mebel A.M.; Editors  
International Conference on Physics and Chemistry of Combustion and Processes in Extreme Environments (COMPHYSCHEM'20-21) and VI International Summer School "Modern Quantum Chemistry Methods in Applications" held in Samara, Russia 26-30 July 2021.  
AIP Conf. Proc., 2020; 2304(1).

## Presentations--Alexander M. Mebel

1. "Theoretical Study of Structure and Structural Non-Rigidity of Boron Hydrides  $B_n$  ( $n = 6-12$ )"  
A.M. Mebel and O.P. Charkin  
International Congress on Quantum Chemistry, Tatranska Lomnice, Czechoslovakia, Oct. 5-9, 1988.
2. "Theoretical Study of the Reaction of the  $H_2$  Molecule Cleavage from the  $B_6$  and  $AlB_5$  Anions"  
A.M. Mebel and O.P. Charkin  
International Conference on Chemical Reactivity and Elementary Processes, Prague, Czechoslovakia, Sep. 7-10, 1989.
3. "Ab initio MO Study of Structure, Stability and Rearrangement in Iridaborane,  $[(IrB_5H_8)(CO)(PH_3)_2]$ "  
A.M. Mebel, N. Koga and K. Morokuma  
The Third World Congress of Theoretical Organic Chemists, Toyohashi, Japan, Jul. 18-24, 1993.
4. "Ab Initio MO Study of Potential Energy Surfaces for the  $NH + NO_2$  and  $HNO + NO$  Reactions"  
A.M. Mebel, K. Morokuma and M.C. Lin  
Twenty-Third Southeastern Theoretical Chemistry Association Conference, Vanderbilt University, Tennessee, May 20-21, 1994.
5. "Ab Initio MO Calculations of Potential Energy Surface of the  $HNO + NO$  Reaction"  
A.M. Mebel, K. Morokuma, M.C. Lin and C.F. Melius  
Gordon Research Conf. on Energetic Materials, New Hampton, NH, Jun. 26-Jul. 1, 1994.
6. "Ab Initio MO Calculations of the Thermochemistry of the ADN System"  
A.M. Mebel, K. Morokuma and M.C. Lin  
Gordon Research Conf. on Energetic Materials, New Hampton, NH, Jun. 26-Jul. 1, 1994.
7. "Ab Initio Molecular Orbital Study of Potential Energy Surface for the  $HNO + NO$  Reaction"  
A.M. Mebel, K. Morokuma and M.C. Lin  
American Chemical Society 46th SE Regional Meeting, Birmingham, AL, Oct. 16-19, 1994.
8. "Theoretical Study of the Gas Phase Structure, Thermochemistry and Decomposition Mechanisms of  $NH_4NO$  and  $NH_4N(NO_2)_2$  (ADN)."  
A.M. Mebel, M.C. Lin and K. Morokuma  
1994 Fall Technical Meeting. The Eastern States Section of Combustion Institute, Clearwater Beach, FL, Dec. 5-7, 1994.

9. "Ab initio and RRKM calculations for the multichannel rate constants of the  $C_2H_3 + O_2$  reaction."  
A.M. Mebel, E. W.-G. Diau, M.C. Lin and K. Morokuma  
1995 Fall Technical Meeting. The Eastern States Section of Combustion Institute, Worcester, MA, Oct. 16-18, 1995.
10. "Theoretical rate constants for the  $NH_3 + NO_x \rightarrow NH_2 + HNO_x$  ( $x = 1,2$ ) reactions by ab initio MO/VTST calculations."  
A.M. Mebel, E. W.-G. Diau, M.C. Lin and K. Morokuma  
1995 Fall Technical Meeting. The Eastern States Section of Combustion Institute, Worcester, MA, Oct. 16-18, 1995.
11. "The  $CH_3 + C_5H_5$  reaction: a potential source of benzene at high temperatures."  
Moskaleva L.V., Mebel A.M., Lin M.C.  
Twenty Sixth Symposium (International) on Combustion, Naples, Italy, July 28 - August 2, 1996.
12. "Thermal reduction of NO by  $NH_3$ : kinetic modeling of the  $NH_2 + NO$  product branching ratio."  
Halbgewachs M.J., Diau E.W.G., Mebel A.M., Lin M.C., Melius C.F.  
Twenty Sixth Symposium (International) on Combustion, Naples, Italy, July 28 - August 2, 1996.
13. "Theoretical study of vibronic spectra of methyl radical and methane. Photodissociation pathways of methane."  
Mebel A.M., Lin S.H., Chang C.-H.  
International Symposium "Modern Trends in Chemical Dynamics", Taipei, Taiwan, December 8-12, 1996.
14. "Ab initio calculations of vibronic coupling. Applications to symmetry-forbidden vibronic spectra and internal conversion of ethylene."  
Mebel A.M., Hayashi M., Lin S.H.  
7th Asian Chemical Congress, Hiroshima, Japan, May 16-20, 1997.
15. "Using ab initio MO calculations to understand the photodissociation dynamics of  $C_3H_4$  and  $C_3H_2$ ."  
Mebel A.M., Jackson W.M., Lin S.H., Lee Y.T.  
9th International Congress of Quantum Chemistry, Atlanta, Georgia, USA, June 9-14, 1997.
16. "Applications of ab initio molecular orbital calculations to electronic spectroscopy and photodissociation dynamics of small organic molecules and radicals"  
Mebel A.M., Hayashi M., Lin S.H.  
Gordon Research Conference on Molecular Spectroscopy and Dynamics, Oxford, UK, September 1-5, 1997.

17. "Theoretical studies of photochemistry of C<sub>2</sub>H<sub>4</sub>: vibronic spectra, the rates of internal conversion, and photodissociation rate constants"  
Mebel A.M.  
2nd Japan-Taiwan Workshop on Chemical Kinetics,  
Chi-tou, Taiwan, March 18-20, 1998.
18. "Theoretical studies of photochemistry of C<sub>2</sub>H<sub>4</sub>: vibronic spectra, the rates of internal conversion, and photodissociation rate constants"  
Mebel A.M., Chang A.H.H., Hayashi M., Lin S.H.  
13th Canadian Symposium on Theoretical Chemistry,  
Vancouver, Canada, August 2-7, 1998.
19. "Ab initio calculations of potential energy surfaces with applications to the studies of photochemical and crossed molecular-beam reactions"  
Mebel A.M.  
French-Taiwanese Workshop "Molecular Dynamics and Dynamics of Alkali/Hydrogen Reactions",  
Orsay, France, October 12-14, 1998.
20. "Ab initio calculations of symmetry-forbidden vibronic spectra: The n- $\pi^*$  electronic transition in acetone"  
Mebel A.M., Liao D.-W., Hayashi M., Shiu Y.J., Chen Y.T., Lin S.H.  
In the Frontiers of Quantum Chemistry and Chemical Reactions,  
Atlanta (Georgia, USA) in May 21-22, 1999.
21. "Ab Initio Studies of Symmetry-Forbidden Vibronic Spectra and Rates of Internal Conversion in Polyatomic Molecules"  
Mebel A.M., Hayashi M., Lin S.H.  
5th World Congress of Theoretically Oriented Chemists  
London, UK, August 1-6, 1999
22. "Ab initio calculations of vibronic spectra and dynamics of small polyatomic molecules: Role of Duschinsky effect"  
Mebel A.M., Hayashi M., K.K. Liang, Lin S.H.  
Workshop on Computational Chemistry  
Hong Kong, February 21-24, 2000.
23. "Ab initio study of branching ratios of C<sub>2</sub> products in the photodissociation of C<sub>2</sub>H at 193 nm" (Invited Lecture)  
Mebel A.M., Hayashi M., Jackson W.M., Lin S.H.  
13<sup>th</sup> European Conference on Dynamics of Molecular Collisions. MOLEC  
2000  
Jerusalem, Israel, September 17-22, 2000.

24. "Theoretical prediction of reaction rate constants and product branching ratios from ab initio calculations: Applications to various reactions in combustion and atmospheric chemistry" (Invited Lecture) Mebel A.M., Lin M.C., Lee H.Y., Kaiser R.I., Lee Y.T., Hayashi M., Lin S.H., 2000 International Chemical Congress of Pacific Basin Societies  
Honolulu, Hawaii, USA, December 14-19, 2000.
25. "Theoretical prediction of reaction rate constants and product branching ratios from ab initio calculations: Reactions in combustion and atmospheric chemistry" (Invited Lecture)  
Mebel A.M.  
5<sup>th</sup> East Asian Workshop on Chemical Reactions  
Sendai, Japan, March 23-25, 2001.
26. "Product branching ratios of the  $C(^3P) + C_2H_3(^2A')$  and  $CH(^2\Pi) + C_2H_2(^1\Sigma_g^+)$  reactions and photodissociation of  $H_2CC\equiv CH(^2B_1)$  at 193 and 242 nm: An ab initio/RRKM study"  
Nguyen T.L., Mebel A.M., Lin S.H., Kaiser R.I.  
Faraday Discussion 119, Combustion Chemistry: Elementary Reactions to Macroscopic Processes  
University of Leeds, Leeds, UK, July 9-11, 2001.
27. "Ab initio calculations of potential energy surfaces, reaction rate constants and product branching ratios: Applications to combustion and atmospheric chemistry" (Invited Lecture)  
Mebel A.M.  
XIII Symposium on Modern Chemical Physics, Tuapse-2001  
Tuapse, Russia, September 25 – October 5, 2001.
28. "Theoretical study of closo borane, alane, and gallane icosahedral clusters with noble gas atoms and cations of light atoms inside and outside of cluster cage"  
Mebel A.M., Charkin O.P., Klimenko N.M., Moran D., Charkin O.D., Schleyer P.v.R.  
Gordon Conference on Molecular and Ionic Clusters  
Ventura, California, January 6-11, 2002.
29. "Ab initio/RRKM study of dissociation pathways of benzene trication: an approach to understanding Coulomb explosion of benzene"  
Mebel A.M.  
Academia Sinica – Israel Academy of Sciences and Humanities Meeting.  
Chemical Dynamics: From Small Molecules to Biomolecules  
Taipei, Taiwan, May 9-10, 2002.
30. "Ab initio/RRKM studies of the reactions of atomic carbon and oxygen with hydrocarbon molecules: Synergism between theory and crossed molecular beam experiments", Mebel A.M., 6th World Congress of Theoretically Oriented Chemists (WATOC-02), Lugano, Switzerland, August 4-9, 2002.

31. "Application of the ab initio/RRKM approach to photodissociation of 1,2- and 1,3-butadienes and 2-butyne at 193 nm: Product branching ratios (Invited Lecture)  
Lee H.Y., Kislov V.V., Lin S.H., Mebel A.M., Neumark D.M., Second Worldwide Chinese Theoretical and Computational Chemistry Conference (WCTCC 2002)  
Taipei, Taiwan, September 2-7, 2002.
32. "A theoretical study of isomerism in doped aluminum MAI<sub>12</sub> and MAI<sub>12</sub>X<sub>12</sub> clusters with 40 and 50 valence electrons"  
Charkin O.P., Charkin D.O., Klimenko N.M., Mebel A.M.  
Faraday Discussion #124  
York, UK, April 14-16, 2003.
33. "Quantum chemical modeling of photoluminescence properties of silica-based nanoscale materials"  
Zyubin A.S., Mebel A.M., Glinka Yu.D., Lin S.H.  
Faraday Discussion #124  
York, UK, April 14-16, 2003.
34. "Theoretical prediction of reaction rate constants and product branching ratios in photodissociation and Coulomb explosion reactions" (Invited Lecture)  
Mebel A.M.  
7<sup>th</sup> East Asian Workshop on Chemical Reactions  
Taipei, Taiwan, March 27-29, 2003.
35. "Prediction of reaction rate constants and product branching ratios using ab initio potential energy surfaces in combination with RRKM and radiationless transition theories"  
Mebel A.M., Kislov V.V., Hayashi M., Lin S.H.  
228<sup>th</sup> ACS National Meeting, Philadelphia, PA, August 22-26, 2004.
36. "Potential energy surfaces in Coulomb explosion of polyatomic molecules in the presence and absence of external electric field" (Invited Lecture)  
Mebel A.M., Zyubina T.S., Dyakov Y.A., Lin S.H., Bandrauk A.D.  
Pacifichem 2005, Honolulu, Hawaii, December 15-20, 2005.
37. "Theoretical studies of the C<sub>5</sub>H<sub>4</sub> potential energy surfaces and reaction mechanisms of C<sub>2</sub> with C<sub>3</sub>H<sub>4</sub>"  
Mebel A.M., Kislov V.V., Kaiser R.I.  
Pacifichem 2005, Honolulu, Hawaii, December 15-20, 2005.
38. "Matrix isolation of unstable intermediates in astrophysically relevant ices"  
Jamieson C.S., Bennett C.J., Mebel A.M., Kaiser R.I.  
Pacifichem 2005, Honolulu, Hawaii, December 15-20, 2005.
39. "An ab initio G3-type study of the indene formation pathways", Kislov V.V., Mebel A.M., 232<sup>nd</sup> ACS National Meeting, San Francisco, California, September 10-14, 2006.

40. "Matrix isolation study of high-order carbon oxides ( $\text{CO}_n$ ,  $n = 3-5$ )" Jamieson C.S., Mebel A.M., Kaiser R.I., 232<sup>nd</sup> ACS National Meeting, San Francisco, California, September 10-14, 2006.
41. "Theoretical studies of potential energy surfaces, rate constants, and product branching ratios for the reactions of  $\text{C}_2$  and  $\text{C}_3$  with unsaturated hydrocarbons" (Invited Lecture), Mebel A.M., Kislov V.V., Kaiser R.I., 232<sup>nd</sup> ACS National Meeting, San Francisco, California, September 10-14, 2006.
42. "Theoretical studies of the potential energy surface and mechanism of the  $\text{C}_2\text{H}(^2\Sigma^+) + \text{C}_4\text{H}_2(^1\Sigma_g^+) \rightarrow \text{C}_6\text{H}_2 + \text{H}$  reaction" (Invited Talk) Mebel A.M., Landera A., Kislov V.V. First Workshop on 'Titan – Observations, Experiments, Computations and Modeling', Honolulu, Hawaii, February 5-7, 2007.
43. "Theoretical studies of the mechanism and kinetics of elementary combustion and interstellar reactions" (Invited Talk) Mebel A.M., Kislov V.V. Joint Symposiums on Chemical Kinetics and Renewable Energy: From Gas Phase to Condensed Phase, Hsinchu, Taiwan, June 5-9, 2007.
44. "Theoretical studies of reactions of ethynyl radical with unsaturated hydrocarbons related to the growth of organic molecules in Titan's atmosphere" (Invited Talk) Landera A., Krishtal S. P., Kislov V.V., Mebel A.M. Joint Symposium on Computational Chemistry, Hanoi, Vietnam, December 21-22, 2007.
45. "Theoretical studies of reactions of ethynyl radical with unsaturated hydrocarbons related to the growth of organic molecules in Titan's atmosphere" (Invited Talk) Landera A., Krishtal S. P., Kislov V.V., Mebel A.M. Second Workshop on 'Titan – Observations, Experiments, Computations, and Modeling', Miami, Florida, March 24-26, 2008.
46. "Toward the formation of Titan's aerosol layers" Zhang F., Gu X., Zhou L., Mebel A.M., Kaiser R.I., Second Workshop on 'Titan – Observations, Experiments, Computations, and Modeling', Miami, Florida, March 24-26, 2008.
47. "H elimination and metastable lifetimes in the UV photoexcitation of diacetylene" Silva R., Gichihi W.K., Huang C., Doyle M.B., Kislov V.V., Mebel A.M., Suits A.G., Second Workshop on 'Titan – Observations, Experiments, Computations, and Modeling', Miami, Florida, March 24-26, 2008.
48. "An ab initio G3-type/statistical theory study of naphthalene and indene formation pathways originated from reactions of cyclopentadiene and cyclopentadienyl radical" Kislov V.V., Mebel A.M., 235<sup>th</sup> ACS National Meeting, New Orleans, Louisiana, April 6-10, 2008.
49. "Theoretical studies of chemical reactions of astrochemical relevance" Mebel A.M., Kislov V.V., Kaiser R.I., Gordon Research Conference on Atomic and Molecular Interactions, New London, NH, July 6-11, 2008.

50. "Cold fusion' to PAH: A novel photoinduced ethynyl addition mechanism of the formation and growth of polycyclic aromatic hydrocarbons in low-temperature environments" Mebel A.M., Kislov V.V., Kaiser R.I., Dynamics and Spectroscopy of Small Molecules and Biomolecules, Taipei, Taiwan, November 9-12, 2008.
51. "Reaction mechanisms for the formation and growth of aromatic molecules in Titan's atmosphere" Mebel A.M., Kislov V.V., Jamal A., Kaiser R.I., Third Workshop on 'Titan – Observations, Experiments, Computations, and Modeling', San Juan, Puerto Rico, February 26-28, 2009.
52. "Theoretical studies of the reaction mechanism and product branching ratios of  $C_2H + C_2H_4$  and related reactions: The production of vinylacetylene" Krishtal S.P., Mebel A.M., Third Workshop on 'Titan – Observations, Experiments, Computations, and Modeling', San Juan, Puerto Rico, February 26-28, 2009.
53. "Theoretical studies of the kinetics of reactions of importance in Titan's atmospheric chemistry" Klippenstein S.J., Harding L.B., Kislov V.V., Mebel A.M., Third Workshop on 'Titan – Observations, Experiments, Computations, and Modeling', San Juan, Puerto Rico, February 26-28, 2009.
54. "Photodissociation of diacetylene dimer and hydrocarbon growth in Titan's atmosphere" Huang C., Zhang F., Kaiser R.I., Kislov V.V., Mebel A.M., Silva R., Gichuhi W.K., Suits A.G., Third Workshop on 'Titan – Observations, Experiments, Computations, and Modeling', San Juan, Puerto Rico, February 26-28, 2009.
55. "Growth mechanisms of large organic molecules in low-temperature conditions of Titan's atmosphere: from polyynes to PAH" Mebel A.M., Kislov V.V., Landera A., Jamal A., Kaiser R.I., International Symposium on Theory of Molecular Structure and Reactivity, Kyoto, Japan, July 19-21, 2009.
56. "Theoretical study of the reaction mechanism and product branching ratios of the reactions of ethynyl radical with allene and methylacetylene in Titan's atmosphere" Mebel A.M., Jamal A., 239th ACS National Meeting, San Francisco, CA, US, March 21-25, 2010.
57. "Theoretical study of the mechanism, rate constants, and product branching ratios for the reaction of phenyl radical with 1,2-butadiene at different temperatures and pressures" Kislov V.V., Mebel A.M., 239th ACS National Meeting, San Francisco, CA, US, March 21-25, 2010.
58. "Homogeneous and heterogeneous hydrocarbon chemistry in Titan's atmosphere" Jones B., Zhang F., Maksyutenko P., Mebel A.M., Kaiser R.I., 239th ACS National Meeting, San Francisco, CA, US, March 21-25, 2010.
59. "Primary photodissociation dynamics of hydrocarbons relevant to Titan's atmosphere" Suits A.G., Huang C., Gichuhi W., Silva R., Kislov V.V., Zhang F., Mebel A.M., Kaiser R.I., 239th ACS National Meeting, San Francisco, CA, US, March 21-25, 2010.

60. "Mechanisms of Formation of Nitrogen-Containing Polycyclic Aromatic Compounds in Low-Temperature Environments of Planetary Atmospheres: A Theoretical Study" Landera A., Mebel A. M., Faraday Discussion 147, Chemistry of Planets, Saint Jacut de la Mer, Brittany, France, June 14-16, 2010.
61. "Addition of one and two units of C<sub>2</sub>H to styrene: A theoretical study of the C<sub>10</sub>H<sub>9</sub> and C<sub>12</sub>H<sub>9</sub> systems and implication towards Titan's atmosphere" Landera A., Mebel A.M., Kaiser R.I., Faraday Discussion 147, Chemistry of Planets, Saint Jacut de la Mer, Brittany, France, June 14-16, 2010.
62. "An ab initio/RRKM study of the reaction mechanism and product branching ratios of ethynyl radical (C<sub>2</sub>H) with unsaturated hydrocarbons" Jamal A., Mebel A.M., Faraday Discussion 147, Chemistry of Planets, Saint Jacut de la Mer, Brittany, France, June 14-16, 2010.
63. "Primary photodissociation processes important in Titan's atmosphere" Gichuhi W., Huang C., Zhang F., Kaiser R.I., Kislov V.V., Mebel A.M., Silva R., Suits A.G., Faraday Discussion 147, Chemistry of Planets, Saint Jacut de la Mer, Brittany, France, June 14-16, 2010.
64. "Isomer-specific spectroscopy of gas-phase 1-hydronaphthyl, 2-hydronaphthyl, and 1,2,3-trihydronaphthyl radicals" Sebree J.A., Zwier T.S., Kislov V.V., Mebel A.M., Faraday Discussion 147, Chemistry of Planets, Saint Jacut de la Mer, Brittany, France, June 14-16, 2010.
65. "Theoretical studies of reaction mechanisms of C<sub>2</sub>H with unsaturated hydrocarbons in Titan's atmosphere" Mebel A.M., Landera A., Jamal A., Kaiser R.I., 4<sup>th</sup> NSF Workshop on Titan "Observations, Experiments, Computations and Modeling", Saint Jacut de la Mer, France, June 16-18, 2010.
66. "Theoretical studies of reaction mechanisms relevant to hydrocarbon growth in Titan's atmosphere" Mebel A.M., Jamal A., Landera A., Kaiser R.I., 5<sup>th</sup> NSF Workshop on Titan "Observations, Experiments, Computations and Modeling", Poipu Koloa, Kauai, Hawaii, April 11-14, 2011.
67. "An ab initio RRKM study of the mechanism and product branching ratios in the reactions of ethynyl radical with C<sub>4</sub>H<sub>6</sub> isomers" Jamal A., Mebel A.M., 5<sup>th</sup> NSF Workshop on Titan "Observations, Experiments, Computations and Modeling", Poipu Koloa, Kauai, Hawaii, April 11-14, 2011.
68. "A theoretical study of the potential energy surface for the C<sub>2</sub> + C<sub>4</sub>H<sub>4</sub> → C<sub>6</sub>H<sub>3</sub> + H reaction" Landera A., Mebel A.M., 5<sup>th</sup> NSF Workshop on Titan "Observations, Experiments, Computations and Modeling", Poipu Koloa, Kauai, Hawaii, April 11-14, 2011.

69. "Ab initio/RRKM study of the reaction mechanism and product branching ratios of cyano radical (CN) with C<sub>4</sub>H<sub>6</sub> isomers" Jamal A., Mebel A.M., 242nd ACS National Meeting & Exposition, Denver, CO, United States, August 28 – September 1, 2011.
70. "Addition of vinylacetylene (C<sub>4</sub>H<sub>4</sub>) to phenyl radical (C<sub>6</sub>H<sub>5</sub>): A theoretical and kinetic investigation towards the formation of naphthalene in combustion flames" Landera A., Mebel A.M., 242nd ACS National Meeting & Exposition, Denver, CO, United States, August 28 – September 1, 2011.
71. "Reaction mechanisms of the growth of complex organic molecules including PAH in Titan's atmosphere: A view from theoretical calculations of potential energy surfaces" Mebel A.M., Jamal A., Landera A., Kislov V.V., Kaiser R.I., 6th Workshop on Titan Chemistry 'Observations, Experiments, Computations, and Modeling', Miami, Florida, March 12-14, 2012.
72. "Theoretical study of the reaction mechanism and product branching ratios of ethynyl and cyano radical with unsaturated hydrocarbons on Titan" Jamal A., Mebel A.M., 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-March 29, 2012.
73. "Reaction Mechanisms of the Growth of Aromatic and Polycyclic Aromatic Hydrocarbons in Titan's Atmosphere: A View from Theoretical Calculations of Potential Energy Surfaces" Mebel A.M., Jamal A., Landera A., Kislov V.V., Kaiser R.I., Astrobiology Science Conference, Atlanta, Georgia, April 16-20, 2012.
74. "Theoretical studies of chemical reactions related to the formation and growth of polycyclic aromatic hydrocarbons and molecular properties of their key intermediates", Mebel A.M., 33<sup>rd</sup> Annual Combustion Research Meeting, Potomac, Maryland, May 29 – June 1, 2012.
75. "Reaction mechanisms of the growth of polycyclic aromatic hydrocarbons and nitrogen-containing polycyclic aromatic compounds at low temperatures: A view from theoretical calculations of potential energy surfaces", Landera A., Kislov V.V., Kaiser R.I., Mebel A.M., Faraday Discussion 157, Assisi, Italy, June 25-27, 2012.
76. "Combined photodissociation and pyrolysis study of the dissociation mechanisms of ortho benzyne: A theoretical point of view", Landera A., Mebel A.M., 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012, PHYS-320.
77. "Formation of Gas-Phased Aromatics From Ethynyl Radical in the Interstellar Medium (ISM) and Planetary Systems: An Ab Initio Quantum Chemical & RRKM Study", Jamal A., Mebel A.M., 68th Southwest Regional Meeting of the American Chemical Society, Baton Rouge, LA, United States, November 4-7, 2012, SWRM-380.

78. "Theoretical studies of the reactions of dicarbon (C<sub>2</sub>) with C<sub>3</sub>H<sub>6</sub> and C<sub>4</sub>H<sub>6</sub> and their implications in combustion and astrochemistry", Landera A., Mebel A.M., 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013, PHYS-412.
79. "HACA mechanism revised: Formation of PAHs beyond the second aromatic ring", Kislov V.V., Mebel A.M., 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013, PHYS-79.
80. "Formation of the first aromatic ring in cold planetary atmospheres and the ISM: An ab initio/RRKM study", Jamal A., Mebel A.M., 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013, COMP-390.
81. "Ab initio/RRKM studies of the reactions of dicarbon (C<sub>2</sub>) with C<sub>3</sub>H<sub>6</sub> and C<sub>4</sub>H<sub>6</sub> and their implications in combustion and astrochemistry", Mebel A.M., Landera A., 89<sup>th</sup> Florida Annual Meeting and Exposition (FAME 2013) of FLACS, Innisbrook Resort and Golf Club, May 9-11, 2013.
82. "Photochemically induced cold synthesis of complex organic molecules on Titan and in the interstellar medium: A view from ab initio/RRKM calculations", Mebel A.M., 6<sup>th</sup> World Congress of Chinese Theoretical and Computational Chemists (WCTCC6), Tamkang University, Taiwan, June 24-28, 2013.
83. "Photochemically induced cold synthesis of complex organic molecules on Titan and in the interstellar medium: A view from ab initio/RRKM calculations", Mebel A.M., International Conference on Chemical Bonding, Kauai, Hawaii, USA, July 4-8, 2013.
84. "Ab initio/RRKM studies of the reactions of dicarbon (C<sub>2</sub>) with C<sub>3</sub>H<sub>6</sub> and C<sub>4</sub>H<sub>6</sub> and their implications in combustion and astrochemistry", Landera A., Kaiser, R.I., Mebel A.M., 32<sup>nd</sup> International Symposium on Free Radicals, Potsdam, Germany, July 21-26, 2013.
85. "Reaction Mechanisms of the Growth of Nitrogen-Containing Polycyclic Aromatic Compounds at Low Temperatures: A View from Theoretical Calculations of Potential Energy Surfaces", Landera A., Mebel A.M., 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013.
86. "Reaction mechanisms between CH (X<sup>2</sup>Π) and CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, and C<sub>2</sub>H<sub>6</sub>: An ab initio study", Ribeiro J.M.L., Mebel A.M., 247th ACS National Meeting & Exposition, Dallas, TX, United States, March 16-20, 2014.
87. "Roaming Mechanism in Cl Radical Addition-Elimination Reactions with Alkenes", Joalland B., Shi Y., Kamasah A., Suits A.G., Mebel A.M., 23<sup>rd</sup> International Symposium on Gas Kinetics and Related Phenomena, Szeged, Hungary, July 21-24, 2014.

88. "Roaming Mechanism in Cl Radical Addition-Elimination Reactions with Alkenes", Joalland B., Shi Y., Kamasah A., Suits A.G., Mebel A.M., International Conference on Chemical Bonding, Kauai, Hawaii, July 24-28, 2014.
89. "Rate coefficients and product branching ratios for the oxidation of phenyl and naphthyl radicals: A theoretical RRKM-ME study", Kislov V.V., Singh R.I., Edwards D. E., Mebel A. M., Frenklach M., 35th International Symposium on Combustion, San Francisco, August 4-8, 2014.
90. "Low temperature dynamics and kinetics of the bimolecular reactions between CH ( $X^2\Pi$ ) and CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>: An ab initio study", Ribeiro J.M.L., Mebel A.M., 248th National Meeting of the American Chemical Society, San Francisco, CA, August 10-14, 2014, 554-PHYS.
91. "Bimolecular reactions of dicarbon radicals with C<sub>3</sub>, C<sub>4</sub>, and C<sub>5</sub> unsaturated hydrocarbons: Energetics and dynamics of combustion intermediates", Dangi B.B., Parker D.S., Kaiser R., Landera A., Belisario-Lara D., Mebel A.M., 250th ACS National Meeting & Exposition, Boston, MA, United States, August 16-20, 2015, PHYS-20.
92. "Reaction mechanisms and branching ratios between CH ( $X^2\Pi$ ) and C<sub>3</sub>H<sub>8</sub>, C<sub>3</sub>H<sub>6</sub> and C<sub>3</sub>H<sub>4</sub>: An ab initio study", Ribeiro J.M.L., Mebel A.M., 250th ACS National Meeting & Exposition, Boston, MA, United States, August 16-20, 2015, PHYS-559.
93. "Mechanisms of PAH growth and oxidation in combustion", Mebel A.M., Reaction Dynamics Symposium Commemorating IAMS 20th Anniversary, Taipei, Taiwan, November 10-12, 2015.
94. "Mechanisms of PAH growth and oxidation in combustion", Mebel A.M., 56th Sanibel Symposium, St. Simons Island, Georgia, February 15-19, 2016.
95. "Temperature- and Pressure-Dependent Rate Coefficients for the HACA Pathways from Benzene to Naphthalene", Mebel A.M., Georgievskii Y., Jasper A.W., Klippenstein S.J., 36<sup>th</sup> International Symposium on Combustion, Seoul, Korea, July 31 – August 5, 2016.
96. "Pressure Dependent Rate Constants for PAH Growth: Formation of Indene and its Conversion to Naphthalene", Mebel A.M., Georgievskii Y., Jasper A.W., Klippenstein S.J., Faraday Discussion on Reaction Rate Theory, Cambridge, UK, September 19-21, 2016.
97. "Mechanism and rate constants for PAH growth and oxidation in combustion", Mebel A.M., 7th International Symposium on Nonequilibrium Processes, Plasma, Combustion and Atmospheric Phenomena (NEPCAP 2016), Sochi, Russia, October 2-7, 2016.

98. "A Combined Molecular Beams and Computational Study on the Decomposition of JP-8 & JP-10 Jet Fuel -From Surrogates to Real Fuel", Kaiser R.I., Mebel A.M., MACCCR Meeting, Chicago, IL, Oct. 18-21, 2016.
99. "Investigation on pyrolysis of jet propellant 8", Belisario-Lara, D., Mebel A.M., 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017, PHYS-489.
100. "Trivalent f-metal coordination and extraction by tripodal sulfonamide ligands and analogs", Govor E.V., Anagnostopoulos V.A., Morozov A.N., Mebel A.M., Raptis R.G., Kavallieratos, K., 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017 (2017), INOR-1138.
101. "Kinetic, product, and computational studies of the ultrasonically induced degradation of 4-methylcyclohexanemethanol (MCHM)", Cui, D., Mebel A.M., Arroyo-Mora L.E., Holness H., Furton K., O'Shea K.E., 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017, ENVR-510.
102. "Structural, spectroscopic, and theoretical studies on the effects of pyrazole substitution and ion-pairing in binding and sensing of  $\text{NH}_4^+$  and Lanthanides(III) by tripodal tris-pyrazole receptors", Jonah T.M., Govor E.V.; Kandel S., Mathivathanan L., Raptis R.G., Morozov A.N.; Mebel A.M.; Kavallieratos, K., 254th ACS National Meeting & Exposition, Washington, DC, USA, August 20-24, 2017 (2017), I+EC-21.
103. "Theoretical study on pyrolysis of Jet Propellant-8 components: The behavior of aliphatic and non-aliphatic alkyl rings", Belisario-Lara D., Mebel A., Ribeiro J.M., 254th ACS National Meeting & Exposition, Washington, DC, USA, August 20-24, 2017 (2017), COMP-165.
104. "Recent advances in theoretical studies of reaction mechanisms and rate constants of PAH oxidation and growth in combustion", Keynote Presentation, Mebel A.M., International Conference on Aerospace Technology, Communications, and Energy Systems (ATCES), Samara, Russia, September 28-30, 2017.
105. "Reaction mechanisms and rate constants of PAH growth in astrophysical environments", Mebel A.M., 255th ACS National Meeting & Exposition, New Orleans, LA, United States, March 18-22, 2018 (2018), PHYS-192.
106. "Reaction mechanisms and rate constants of PAH growth in astrophysical environments", Mebel A.M., FAME 2018, Palm Harbor, FL, USA, May 3-5, 2018.
107. "The mechanism and kinetics of oxidation of cyclopentadienyl radical in combustion flames: A theoretical view", Ghildina A.R., Oleinikov A.D., Galimova G.R., Azyazov V.N., Mebel A.M., FAME 2018, Palm Harbor, FL, USA, May 3-5, 2018.

108. "Formation and Growth of Polycyclic Hydrocarbons", Mebel A.M., Computational and Theoretical Chemistry Research PI Meeting, Washington, DC, USA, May 22-24, 2018.
109. "The mechanism and kinetics of oxidation of cyclopentadienyl radical in combustion flames: A theoretical view", Ghildina A.R., Oleinikov A.D., Galimova G.R., Azyazov V.N., Mebel A.M., International Conference on Combustion Physics and Chemistry, ComPhysChem'18, Samara, Russia, July 24-27, 2018.
110. "On the low-temperature limit of HACA", Frenklach M.I, Singh R.I., Mebel A.M., 37<sup>th</sup> International Combustion Symposium, Dublin, Ireland, Jul. 29 – Aug. 3, 2018.
111. "Ultrasonic degradation of an emerging perfluoro ether, Gen X", Cui D., Mebel A., O'Shea K., 256<sup>th</sup> ACS National Meeting & Exposition, Boston, MA, United States, August 19-23, 2018, ENVR-112.
112. "Binding and extraction of trivalent lanthanides by tripodal sulfonamides and pyrazoles: structural, theoretical and spectroscopic studies", Govor E.V., Morozov A.N., Jonah T., Flores G.A., Mebel A.M., Raptis R.G., Kavallieratos K., 256<sup>th</sup> ACS National Meeting & Exposition, Boston, MA, United States, August 19-23, 2018, INOR-430.
113. "Reaction mechanisms and rate constants of PAH growth in astrophysical environments", Mebel A.M., The International Workshop of Gas-Phase Kinetics on Interstellar, Atmospheric and Combustion Chemistry, Hefei, China, March 6-9, 2019.
114. "Trisulfonamide and o-sulfonamidophenol ligands as extractants for trivalent actinides from alkaline high-level waste", Adedoyin O.W., Govor E.V., Morozov A.N., Mebel A.M., Chakraborty I., Raptis R.G., Kavallieratos K., 257<sup>th</sup> ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019, I+EC-0120.
115. "Chemical reaction mechanisms and rate constants of the growth of polycyclic aromatic hydrocarbons (PAH) in combustion flames on Earth, in atmospheres of planets and in the interstellar medium", Mebel A.M., Conference "Science of the Future", Sochi, Russia, May 14-17, 2019.
116. "Reaction Mechanisms and Rate Constants of PAH Growth in Astrophysical Environments", Mebel A.M., Physical Chemistry in Russia and Abroad, Chernogolovka, Russia, June 17-19, 2019.
117. "Reaction Mechanisms and Rate Constants of PAH Growth", Mebel A.M., Non-linear phenomena and dynamics of flame propagation, Borovoe (Burabay) National Nature Park, Kazakhstan, September 21-25, 2019.

118. "Novel synthesis of 5-, 6-, or 7-iodoindenes", Howlader A.H., Diaz K., Mebel A.M., Kaiser R., Wnuk S.F., 259th ACS National Meeting & Exposition, Philadelphia, PA, United States, March 22-26, 2020 (2020), ORGN-0332.
119. "Formation of phenanthrenyl radicals via the reaction of acenaphthyl with Acetylene", Savchenkova A.S., Chechet I.V., Matveev S.G., Frenklach M., Mebel A.M., 38<sup>th</sup> International Symposium on Combustion, Virtual via The Adelaide Convention Centre, Australia, January 24-29, 2021.
120. "Theoretical studies of interstellar and circumstellar reactions of the silyldiyne radical", Mebel, A. M., Nikolayev A. A., Krasnoukhov V., Kaiser R., 262nd ACS National Meeting & Exposition, Atlanta, GA, United States, August 22-26, 2021 (2021).
121. "On the synthesis of the astronomically elusive 1-Ethynyl-3-silacyclopropenylidene (c-SiC<sub>4</sub>H<sub>2</sub>) molecule in circumstellar envelopes of carbon-rich asymptotic giant branch stars and its potential role in the formation of the silicontetracarbide chain (SiC<sub>4</sub>)", Yang Z., Doddipatla S., Kaiser R., Nikolayev A. A., Azyazov V. N., Mebel A. M., 262nd ACS National Meeting & Exposition, Atlanta, GA, United States, August 22-26, 2021 (2021).
122. "Formation of Carbonaceous Materials in Deep Space", Mebel A. M., Pacifichem 2021, Honolulu, HI, Dec. 17, 2021.
123. "Low-temperature oxidation mechanism of a six-member aromatic ring", Medvedkov I. A., Porfiriev D. P., Zagidullin M. V., Azyazov V. N., Morozov A. N., Mebel A. M., Pacifichem 2021, Honolulu, HI, Dec. 19, 2021.
124. "Cleavage of an aromatic ring and radical migration", Mebel A.M., Frenklach M., Faraday Discussion: 100 years of the Lindemann mechanism, Oxford, UK, June 22-24, 2022.
125. "Bay capping via acetylene addition to polycyclic aromatic hydrocarbons: Mechanism and kinetics", Tuli L.B., Mebel A.M., Frenklach M., 39<sup>th</sup> International Symposium on Combustion, Vancouver, Canada, July 24-29, 2022.
126. "Crystal structure, Hirshfeld analysis, and DFT calculations of ferromagnetically-coupled CuI<sub>3</sub>-pyrazolato polymorphs", Rue K., Mezei G., Mathivathanan L., Mebel A.M., Raptis R., Abstracts, 73rd Southeastern Regional Meeting of the American Chemical Society, SERMACS 2022, San Juan, Puerto Rico, October 19-22 2022.
127. "On the mechanisms of soot nucleation", Mebel A.M., Morozov A.N., Frenklach M., Asia Pacific Conference of Theoretical and Computational Chemistry, APATCC-10, Quy Nhon, Vietnam, February 19-23, 2023.

128. "Electronic structure calculations of the reaction of the methylidyne radical CH with vinylacetylene H<sub>2</sub>CCHCCH", Galimova G.R., Mebel A.M., 51st Southeast Theoretical Chemistry Association (SETCA) conference, University of South Carolina, Columbia, SC, USA, May 11-13, 2023.
129. "On the mechanisms of soot nucleation", Mebel A.M., Morozov A.N., Frenklach M., International Conference on Chemical Kinetics (ICCK-2023), Hefei, China, June 26-29, 2023.
130. "Gas phase synthesis of coronene through a directed ring annulation framework", Tuli L.B., Mebel, A.M., ACS Fall 2023, San Francisco, CA, United States, 2023.
131. "Ab initio calculations of the reaction of cyclopropane c-C<sub>3</sub>H<sub>6</sub> through insertion by ground state carbon atoms C(<sup>3</sup>P<sub>j</sub>)", Galimova G., Mebel A.M., ACS Fall 2023, San Francisco, CA, United States, 2023.
132. "Computational study of the thermal degradation of perfluoroalkyl ether carboxylic acids", Paultre C.-B., Mebel A.M., O'Shea K.E., ACS Fall 2023, San Francisco, CA, United States, 2023.
133. "Functionalization of pyrimidine and purine to RNA bases via radical substitution reactions: A theoretical study of reaction pathways toward cytosine, uracil, adenine and guanine", Mebel A.M., Laboratory Astrophysics Workshop (ICE 2024), Kawaii, HI, USA, Feb. 18-22, 2024.