

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:

8/14-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	Engineer 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
IAMS Outstanding Publication Award

2002
2003

Publications

Regular Articles

1. Mebel A.M., Zyubina T.S.
Nonempirical calculations of the potential surface and molecular structure of aluminum oxide (Al_2O) 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 ALi_k and 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 ALi_k and ALi_{k+1}^+ lithides.
Zh. Strukt. Khim. 1988, 29, 22-27.
4. Korkin 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 $\text{B}_{10}\text{H}_{11}^-$ 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 Li^+ affinity of the hydrides MH_n , fluorides MF_n , and lithides MLi_n molecules.
Koord. Khim., 1989, 15, 1478-1488.
16. Mebel A.M., Charkin O.P.
Theoretical study of structure of the $AlB_5H_6^{2-}$, CB_5H_6 , $SiB_5H_6^-$ anions and their protonated derivatives $AlB_5H_7^-$, CB_5H_7 , and SiB_5H_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 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 B_6H_5^- and AlB_5H_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 CB_5H_5 and SiB_5H_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 $\text{B}_8\text{H}_8^{2-}$ 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 $\text{B}_n\text{H}_{n-1}^-$ 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., Korkin 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_2SH formation in the reaction of B_2H_6 with SH_2 : Concerted elimination of BH_3 and H_2 from $H_2S \cdot B_2H_6$. 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_6H_{10} borane and $[(IrB_5H_8)(CO)(PH_3)_2]$ 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 $NH+NO_2$ 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 $C_6H_5O_2$ 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 $[\{\text{Rh}_2(\eta^5\text{-C}_5\text{H}_5)_2(\mu\text{-CH}_2)_2\}_2(\mu\text{-S}_4)]^{2+}$ complex.
Inorg. Chem., 1995, 34, 1208-1211.
43. Lin M.C., Mebel A.M.
An ab initio molecular orbital study of the O + C₆H₅O 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 NH₄NO₂ and NH₄N(NO₂)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 C₂H₃ with H₂ 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 NH₂ + NO₂ 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 HCl with ClONO₂ catalyzed by NO₃⁻.
"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 NH₃ + NO_x → NH₂ + 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.
π-π* 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 HCO + O₂ 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]⁺ 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 N₂O 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 C₂H₃ + O₂ 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 $\text{CH}_3 + \text{C}_5\text{H}_5$ 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_3 : kinetic modeling of the $\text{NH}_2 + \text{NO}$ 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 $\text{H} + \text{HONO}$ 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 $\text{C}_6\text{H}_5 + \text{H}_2$ and $\text{C}_6\text{H}_6 + \text{H}$ 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 CH₂CCH₂ and CH₂C₂
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 C₅H₃ + CH₃ 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- π^* electronic transition of the acetone + nH₂O (n=1-3) complexes.
J. Phys. Chem. A, 1997, 101, 9925-9934.
75. Mebel A.M., Lin M.C.
Theoretical studies of reactions of 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 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 C_3H_n ($n = 1-4$) species and the isomerization mechanism of C_3H_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, $B_nH_n^{2-}$ ($n = 13-17$) 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 $C_6H_6 \cdot I_2$ 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 $B_{12}H_{12}^{2-}$. Structure and nonrigidity of $B_{12}H_{13}^-$ and formation of $B_{12}H_{11}^-$ and $B_{24}H_{23}^{3-}$
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 NH_2 with H_2 , H_2O , NH_3 , and 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 NH_2 with alkanes from ab initio G2M/TST calculations
J. Phys. Chem. A, 1999, 103, 2088-2096.
 92. Pinnaduwa 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 $n-C_4H_3$ formation from reaction of $C(^3P_j)$ with allene, H_2CCCH_2 (X^1A_1)
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 $n\text{-}\pi^*$ 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_4H_4 in triplet electronic state and the reactions of $\text{C}(^3\text{P}_j)$ with C_3H_4 (allene and propyne) and $\text{C}_2(\text{a}^3\Pi_u)$ with $\text{C}_2\text{H}_4(\text{X}^1\text{A}_{1g}^+)$
J. Am. Chem. Soc., 2000, 122, 1776-1788.
101. Hwang D.-Y., Mebel A.M.
Theoretical study on the reversible storage of H_2 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 C₂H
J. Chem. Phys., 2000, 112, 10703-10706.
106. Hwang D-Y., Mebel A.M.
Theoretical Study on Reforming of CO₂ 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, spiropentadiene (C₅H₄), spiropentane (C₅H₈) and bicyclo[1.1.0]but-1(3)-ene (C₄H₄): 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 CO₂ 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 N₂O 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 C₄H₆ isomers I: The 1,3-butadiene molecule, H₂CCHCHCH₂ (X¹A')
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 C₄H₆ isomers II: The dimethylacetylene molecule, H₃CCCCH₃ (X¹A_{1g})
J. Chem. Phys., 2000, 113, 9637-9648.
112. Hwang D-Y., Mebel A.M.
Theoretical study on the reversible storage of H₂ by BeS
J. Am. Chem. Soc., 2000, 122, 11406-11410.
113. Hwang D-Y., Mebel A.M.
Reaction mechanism of CO₂ 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 ($c\text{-C}_3\text{H}$; X^2B_2) formation from reaction of $C(^1D)$ with acetylene, $C_2H_2(X^1\Sigma_g^+)$
J. Chem. Phys., 2001, 114, 231-239.
116. Zyubin A.S., Mebel A.M., Chao S.D., Skodje R.T.
Reaction dynamics of $S(^1D) + H_2/D_2$ 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 $X@Al_{12}H_{12}^{2-}$ closo alane and gallane anions with X atoms of inert gases or halogens inside the icosahedral $[Al_{12}]$ and $[Ga_{12}]$ clusters
Russ. J. Inorg. Chem., 2001, 46, 110-120.
119. Nguyen T.L., Le T.N., Mebel A.M.
Thermochemistry of Cyclopentadienylidene ($c\text{-C}_5\text{H}_4$, C_{2v} , 3B_1), Cyclopentadienyl Radical ($c\text{-C}_5\text{H}_5^\bullet$, C_{2v} , 2B_1), and 1,3-Cyclopentadiene ($c\text{-C}_5\text{H}_6$, C_{2v} , 1A_1): 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 $2^2A'$ and $3^2A'$ electronic states of C_2H
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_5H_5 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_3H_4 potential energy surface and the reaction of $C(^3P)$ with ethylene, C_2H_4
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 $C(^3P)$ 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 C_4H_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 C_4HD_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 C_2H 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 C₂ and C₃ 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 CH₃OH:
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(³P_J), with C₂H₄ and C₃H₆ 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(³P) + C₂H₃(²A') and CH(²Π) + C₂H₂(¹Σ_g⁺) reactions and photodissociation of H₂CC≡CH(²B₁) 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 (A₁₂H₁₂²⁻; A = B, Al, Ga) with Endohedral Noble Gas Atoms (Ng = He, Ne, Ar and Kr) and their Lithium Salts (Li[Ng@A₁₂H₁₂]⁻ and Li₂[Ng@A₁₂H₁₂])
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 C₂N 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-C₃(X¹Σ_g⁺) and c-C₃(X³A₂')
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 C₂H 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(³P) + 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_{12} 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 $[A_{12}H_{12}^{2-}]$ ($A = B, Al, Ga$)
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_2H molecule and the $H_2 + H$ 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 $H + H_2$ 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 $C(^3P) + CH_4$ reaction
J. Phys. Chem. A, 2003, 107, 1788-1796.
 182. Billing G.D., Baer M., Mebel A.M.
Absorption cross section of C_2H : 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_2/H_2 conversion to NH_3 : 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 $C(^3P_j)$ 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 $N_2/H_2/BeO$ and $N_2/H_2/FeO$ 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_4 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_{12} and $\text{MAI}_{12}\text{X}_{12}$ 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 $\text{O}(^1\text{D}) + \text{C}_2\text{H}_6$ 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 $[\text{AlO}_4]^-$ 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 $\text{C}_2(\text{X}^1\Sigma_g^+/\text{a}^3\Pi_u) + \text{C}_2\text{H}_2(\text{X}^1\Sigma_g^+)$ 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, B₂O₂ and BS with H₂
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 CH₄ and He₄ into the C₆₀H₃₆, C₆₀H₂₄, C₈₄, and C₆₀ 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 MH₄ hydrides inside the C₆₀H₃₆, C₆₀H₂₄, C₈₄, and C₆₀ 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 C₂H molecule and the H₂+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 $O(^1D) + CO_2$ 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 LA_{12}
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_4 ($Ng = He, Ne, Ar, Kr, Xe$) inside the $C_{60}H_{36}$ and C_{84} 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 $LA_{12}H_{12}$ with Metal Cations Inside and Outside of the Icosahedral Anion $Al_{12}H_{12}^{2-}$
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 $O(^1D) + NH_3$ 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: $(L@Al_{12})_2$ and $(L@Al_{12})(L'@Al_{12})$ 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 $F+H_2$ 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 $\text{Al}_{13}\text{H}_{2n}^-$ ($n=0-6$) with the centered icosahedral Al_{13} 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 (^2P) 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 $\text{N}_2\text{O}(X^1\Sigma^+)$ 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 heme⁺ 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_s symmetric $OCNO(X^2A')$ 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_{84} (D_{6h}) 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 Tetraatomic Molecules inside the C_{70} (D_{5h}) 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 O₂X< 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, C₂(X¹Σ_g⁺), with methylacetylene, CH₃CCH(X¹A₁): 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 NH₃, NH₂D, NHD₂, and ND₃ 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 (H₂CCCCCH₂) 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 ($C_4H(X^2\Sigma^+)$) 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_4H_4 potential energy surface and of the reactions of $C_2(X^1\Sigma_g^+)$ with $C_2H_4(X^1A_{1g}^+)$ and $C(^1D)$ with C_3H_4 (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_{3h} isomer of carbon trioxide (CO_3) 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_2) with D1 acetylene (HCCD): Possible mechanisms for deuterium enrichment in the interstellar D1-butadiynyl radical, $CCCCD(X^2\Sigma^+)$
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 ($\text{H}_2\text{CCCCCCH}$; C_6H_3 (X^2A')) via reactions of tricarbon molecules, $\text{C}_3(X^1\Sigma_g^+)$ 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, $\text{C}_3\text{H}_5(X^2A_1)$, with methylacetylene ($\text{CH}_3\text{CCH}(X^1A_1)$), allene ($\text{H}_2\text{CCCH}_2(X^1A_1)$), 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 $i\text{-C}_4\text{H}_3(X^2A')$ 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 $\text{C}(^3\text{P}) + \text{C}_2\text{H}_2 \rightarrow \text{I-C}_3\text{H} + \text{H/c-C}_3\text{H} + \text{H/C}_3 + \text{H}_2$ 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_5H_5 - C_5H_4 (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, $C_3(X^1\Sigma_g^+)$, with acetylene, $C_2H_2(X^1\Sigma_g^+)$, ethylene, $C_2H_4(X^1A_g)$, and benzene, $C_6H_6(X^1A_{1g})$ 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_s symmetric isomer of carbon hexaoxide (CO_6) 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_5 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_2CCCH_2) to hexapentaene ($H_2CCCCCCH_2$)
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_6H_3 potential energy surface and rate constants and product branching ratios of the $C_2H(^2\Sigma^+) + C_4H_2(^1\Sigma_g^+)$ and $C_4H(^2\Sigma^+) + C_2H_2(^1\Sigma_g^+)$ 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_8H_7 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 β - and ϵ -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 ($\text{H}-(\text{C}\equiv\text{C})_n-\text{H}$; $n = 1-9$)
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_{10}H_n , $n = 8-12$: 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 $^{32}\text{O}_2/^{36}\text{O}_2$ 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_2H to Styrene: A Theoretical Study of the C_{10}H_9 and C_{12}H_9 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_5H_3 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_2H 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 ($o\text{-C}_6\text{H}_4$) 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 C₆H₃ 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 (C₄H₆). 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 Phenylodiacetylene (C₆H₅CCCCH) and D₅-Phenylodiacetylene (C₆D₅CCCCH) 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., Wnuk 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 C₂H 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 (HCCCC¹¹BO; X¹Σ⁺) via the Reaction of the Boron Monoxide Radical (¹¹BO; X²Σ⁺) with Diacetylene (C₄H₂; X¹Σ_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 (C₂; X¹Σ_g⁺/a³Π_u) with Propene (C₃H₆; X¹A'): 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 (C_6H_5BO) 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 ($C_{14}D_5H_5$; $C_6D_5C_6H_4CCH$) isomers in the reaction of D5-phenyl radicals (C_6D_5 ; X^2A_1) with phenylacetylene ($C_6H_5C_2H$; 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 (C_2H) radicals with unsaturated hydrocarbons acetylene (C_2H_2) and ethylene (C_2H_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 ($C_6H_5CH_2$)
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 (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 ($C_{11}H_{12}$) via the reaction of meta-tolyl (C_7H_7) with 1,3-butadiene (C_4H_6)
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 ($C_{10}H_{10}$) via the reactions of the para-tolyl radical ($C_6H_4CH_3$) with allene (H_2CCCH_2) and methylacetylene ($HCCCH_3$) 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 $CH+CH_4$ 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 $(O_2(a^1\Delta_g))_2$ 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 $Rb(6^2P)$ by H_2 , CH_4 , and C_2H_6
Optics Lett. 2016, 41, 669-672.
384. Ribeiro J.M., Mebel A.M.
Reaction mechanism and product branching ratios of the $CH + C_3H_6$ 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 (C₅O₂) 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 N₃H₃ Isomers in Irradiated Ammonia Bearing Ices: Triazene (H₂NNNH) 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. Int. 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*-C₁₀H₂₂)
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 ($n\text{-C}_{12}\text{H}_{26}$)
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 $\text{Rb}(6^2\text{P})$ with H_2 , CH_4 and C_2H_6
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 $\text{CH} + \text{C}_3\text{H}_4$ 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.
Avoiding Barriers in the Molecular Growth of Polycyclic Aromatic Hydrocarbons - How to Make 1,4-Dihydrophenanthrene at Low Temperatures
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.
 $\text{O}_2(\text{b}^1\Sigma_g^+)$ quenching by O_2 , CO_2 , H_2O , and N_2 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_8H_7) via Triplet Aromatic Cyclooctatetraene (C_8H_8) and Non-Aromatic Cyclooctatriene (C_8H_8) Intermediates Angew. Chem., Int. Ed., 2017, 56, 13655-13660.
405. 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.
406. 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.
407. Krasnoukhov V.S., Porfiriev D.P., Zavershinskiy I.P., Azyazov V.N., Mebel A.M. Kinetics of the $CH_3 + C_5H_5$ Reaction: A Theoretical Study J. Phys. Chem. A, Ahead of Print.
408. Jonah T.M., Mathivathanan L., Morozov A.N., Mebel A.M., Raptis R.G., Kavallieratos, K. Remarkably selective NH_4^+ 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., Ahead of Print.
409. 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., 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.

Presentations--Alexander M. Mebel

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., Hayahi 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 C₂ 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 (O₂)₂ 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 C₂H₆ or CH₄
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 CH₄ and C₂H₆
High Energy/Average Power Lasers and Intense Beam Applications IX, Proceedings of SPIE, Davis S.J., Heaven M.C., Schriempf J.T., Eds.

Presentations--Alexander M. Mebel

v. 9729, Article # 972909, DOI: 10.1117/12.2218119, SPIE-INT Soc. Optical Engineering, Bellingham, WA, USA
San Francisco, CA, Feb. 15-16, 2016.

Presentations--Alexander M. Mebel

1. "Theoretical Study of Structure and Structural Non-Rigidity of Boron Hydrides $B_n H_{n+1}^-$ ($n = 6-12$)"
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 $B_6H_7^-$ and $AlB_5H_7^-$ 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.

Presentations--Alexander M. Mebel

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.

Presentations--Alexander M. Mebel

17. "Theoretical studies of photochemistry of C₂H₄: 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 C₂H₄: 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- π^* 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 C₂ products in the photodissociation of C₂H at 193 nm" (Invited Lecture)
Mebel A.M., Hayashi M., Jackson W.M., Lin S.H.
13th 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.

Presentations--Alexander M. Mebel

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.
5th 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.

Presentations--Alexander M. Mebel

32. "A theoretical study of isomerism in doped aluminum MAI_{12} and $\text{MAI}_{12}\text{X}_{12}$ 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.
7th 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.
228th 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_5H_4 potential energy surfaces and reaction mechanisms of C_2 with C_3H_4 "
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., 232nd ACS National Meeting, San Francisco, California, September 10-14, 2006.
40. "Matrix isolation study of high-order carbon oxides (CO_n , $n = 3-5$)" Jamieson C.S., Mebel A.M., Kaiser R.I., 232nd 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 C_2 and C_3 with unsaturated hydrocarbons" (Invited Lecture), Mebel A.M., Kislov V.V., Kaiser R.I., 232nd ACS National Meeting, San Francisco, California, September 10-14, 2006.

Presentations--Alexander M. Mebel

42. "Theoretical studies of the potential energy surface and mechanism of the $C_2H(^2\Sigma^+) + C_4H_2(^1\Sigma_g^+) \rightarrow C_6H_2 + H$ 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., 235th 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.

Presentations--Alexander M. Mebel

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., Gichihi 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., Gichihi 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_2H to styrene: A theoretical study of the $C_{10}H_9$ and $C_{12}H_9$ 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_2H) with unsaturated hydrocarbons" Jamal

Presentations--Alexander M. Mebel

- 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 C₂H with unsaturated hydrocarbons in Titan's atmosphere" Mebel A.M., Landera A., Jamal A., Kaiser R.I., 4th 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., 5th 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 C₄H₆ isomers" Jamal A., Mebel A.M., 5th 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 C₂ + C₄H₄ → C₆H₃ + H reaction" Landera A., Mebel A.M., 5th 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 C₄H₆ isomers" Jamal A., Mebel A.M., 242nd ACS National Meeting & Exposition, Denver, CO, United States, August 28 – September 1, 2011.
70. "Addition of vinylacetylene (C₄H₄) to phenyl radical (C₆H₅): 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"

Presentations--Alexander M. Mebel

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., 33rd 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 (C₂) with C₃H₆ and C₄H₆ 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 (C₂) with C₃H₆ and C₄H₆ and their implications in combustion and astrochemistry", Mebel A.M., Landera A., 89th 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., 6th World Congress of Chinese

Presentations--Alexander M. Mebel

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_2) with C_3H_6 and C_4H_6 and their implications in combustion and astrochemistry", Landera A., Kaiser, R.I., Mebel A.M., 32nd 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 $CH(X^2\Pi)$ and CH_4 , C_2H_2 , C_2H_4 , and C_2H_6 : 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., 23rd 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_4 , C_2H_6 , C_2H_4 , C_2H_2 : 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_3 , C_4 , and C_5 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_3H_8 , C_3H_6 and C_3H_4 : 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.

Presentations--Alexander M. Mebel

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., 36th 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.