

CURRICULUM VITAE

Alexander M. Mebel

Date and place of birth: May 12, 1961, Simferopol, Ukraine

Country of citizenship: Russia

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:

8/10-present Professor
Department of Chemistry and Biochemistry
Florida International University, Miami, Florida

8/07-8/10 Associate Professor
Department of Chemistry and Biochemistry
Florida International University, Miami, Florida

8/03-8/07 Assistant Professor
Department of Chemistry and Biochemistry
Florida International University, Miami, Florida

10/01-8/03 Associate Research Fellow
Institute of Atomic and Molecular Sciences, Academia Sinica,
Taipei, Taiwan

7/98-9/01 Assistant Research Fellow
Institute of Atomic and Molecular Sciences, Academia Sinica,
Taipei, Taiwan

2/98-6/2000 Visiting Assistant Professor
Tamkang University, Tamsui, Taiwan

1/96-6/98 Senior Academia Sinica Postdoctoral Fellow
Institute of Atomic and Molecular Sciences, Academia Sinica,
Taipei, Taiwan

10/93-12/95 Senior Research Associate
Chemistry Department, Emory University, Atlanta, Georgia, USA

8/92-9/93 Visiting scientist, special researcher
Institute for Molecular Science, Okazaki, Japan.

9/91-3/92 Visiting researcher
Institut für Organische Chemie
Universität Erlangen-Nürnberg, Erlangen, Germany

6/87-2/93 Research worker
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 Lecturer
All-Union Polytechnic Institute
Moscow, Russia

Awards

Academia Sinica Research Award for Junior Researches	2002
IAMS Outstanding Publication Award	2003

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.
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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.
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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.
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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.
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Koord. Khim., 1989, 15, 1155-1161.
 15. Yakobson V.V., Musaev D.G., Zyubin A.S., Mebel A.M., Charkin O.P.
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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.
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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 $(BeH)_k$ ($k = 2, 4, 6$), $A(BeH)_4$, and $A(BeH)_6$.
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.
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21. Mebel A.M., Charkin O.P.
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22. Mebel A.M., Charkin O.P.
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23. Solntsev K.A., Mebel A.M., Votnova N.A., Kuznetsov N.T., Charkin O.P.
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24. Buehl M., Mebel A.M., Charkin O.P., Schleyer P.v.R.
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25. Mebel A.M., Charkin O.P.
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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.
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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.
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J. Phys. Org. Chem., 1995, 8, 407-420.
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Theoretical study of reactions of N_2O with NO and OH radicals.
Int. J. Chem. Kinet., 1996, 28, 693-703.
55. Mebel A.M., Luna A., Lin M.C., Morokuma K.
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J. Chem. Phys., 1996, 105, 9007-9020.
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- J. Phys. Org. Chem., 1996, 9, 801-810.
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75. Hayashi M., Mebel A.M., Liang K.K., Lin S.H.
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Ethylene Photodissociation at 193 and 157 nm
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- Ab initio calculations of vibronic spectra and dynamics for small polyatomic molecules: The role of Duschinsky Effect (Feature Article)
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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.
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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.

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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.
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33. "Quantum chemical modeling of photoluminescence properties of silica-based nanoscale materials"
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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)
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36. "Potential energy surfaces in Coulomb explosion of polyatomic molecules in the presence and absence of external electric field" (Invited Lecture)
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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 "
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38. "Matrix isolation of unstable intermediates in astrophysically relevant ices"
Jamieson C.S., Bennett C.J., Mebel A.M., Kaiser R.I.
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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.

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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.
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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.
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 –

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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.
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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.