CV

Dr. Alexey B. Nadykto

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Education

2012 D.Sc. (Higher Doctorate/Research Professor Dissertation) in Mathematical Modeling (code 05.13.18) and Physical Chemistry (code 02.00.04), awarded by the Academic Qualification Board of the Ministry of Education and Science of Russian Federation.
Dissertation title: Mathematical modeling of the formation of nanoparticles and molecular clusters in nucleating gas-phase media

2001 Ph.D. (Environmental Physics), University of Kuopio, Kuopio, Finland (with Prof. M. Kulmala and A. Laaksonen)
Thesis Title: Nadykto A.B. Condensational growth and evaporation of liquid droplets and ice particles in non-isothermal gas mixtures. *Report Series in Aerosol Science*, 53, 1-65, 2001 (book)

1999 Ph.D. (Physics & Mathematics), L.Karpov Institute of Physical Chemistry, Moscow, Russia (with Prof. E.D. Shchukin)
Thesis Title: The formation and evolution of high temperature aerosols.

1997 M.Sc. (Quantum Physics), Moscow State University, Moscow, Russia (with Prof. G.Ya. Korenman)
Thesis Title: A potential of the interaction between exotic antiprotonic helium atom at long-lived metastable states and helium atom in a gaseous media

Employment

12/2013 – Head of the Laboratory of Molecular Modeling and High-Performance Computations and Principle Scientist/Research Professor, Department of Applied Mathematics, Moscow State University of Technology "STANKIN", Moscow, Russia
02/2010 – Lead Scientist/Research Professor, Department of Applied Mathematics, Moscow State University of Technology "STANKIN", Moscow, Russia
09/2005– Senior Research Scientist, State University of New York, ASRC, Albany, New York, USA
03/2002– 09/2005 Research Scientist, State University of New York, ASRC, Albany, New York, USA
07/2001– 12/2001 Visiting Scientist, University of Helsinki, Department of Physics, Helsinki, Finland
09/1999 – 06/2001 Postdoctoral Fellow of Academy of Finland, University of Kuopio, Department of Applied Physics, Kuopio, Finland
09/1998 – 07/1999 Assistant Professor, Moscow Power Engineering Institute and Moscow State Industrial University, Department of Physics. Moscow.
01/1997 – 02/1999, Ph.D. student, L. Karpov Physico-Chemical Institute, Moscow.

Awards and Fellowships

02/2015 - Entropy Best Paper Award

01/2002-12/2006 Research Fellowship, State University of New York, Albany, NY

01/2001 -12/2001 Fellowship of Nessling Foundation

06/1999-12/2001 Postdoctoral Fellowship of Academy of Finland

Editorial and Other Board Memberships

11/2008 – 12/2014 Central European Journal of Physics (CEJP) (Statistical and Non-Linear Physics)
03/2012 – Expert Council Member, the Committee for Energy, State Duma (Congress) of the Russian Federation http://www.komitet2-13.km.duma.gov.ru/site.xp/051050049.html
04/2011 – Board Member and the Executive Secretary of the Board, Scientific Advisory Board at the Chair of the Committee for Energy, State Duma (Congress) of the Russian Federation;

Research Interests

Kinetics and thermochemistry of gas-to-cluster and cluster-to-bulk phase transitions, structure of molecular clusters and their thermodynamic, spectroscopic and dipolar properties studied using both classical and quantum (*ab initio* and DFT) methods , with a focus on the impact of molecular and nano-scale processes on the evolution of larger nucleating systems

Nucleation theory, including extension of classical (statistical) models and application of quantum methods for solving problems in muticomponent nucleation theory;

Aerosol and nanoparticle microphysics and chemistry

Transport phenomena in disperse systems

Computational Facility and Lab

45 nodes, 8-core Intel Xeon, fully equipped with customized automation system. Accelrys Material Studio 6.0, Gaussian 09, Comsol and other related software, 1 research scientist, 1 postdoctoral fellow, 2 graduate students, 1 research technician.

Publications

1. Alexey B. Nadykto, Jason Herb, Fangqun Yu, YishengXu and Ekaterina S. Nazarenko Estimating the Lower Limit of the Impact of Amines on Nucleation in the Earth's Atmosphere, *Entropy* 2015, *17*, doi:10.3390/e170x000x
2. Nadykto, Alexey B., et al. "Reply to the "Comment on 'Enhancement in the production of nucleating clusters due to dimethylamine and large uncertainties in the thermochemistry of amine-enhanced nucleation"'by Kupiainen-Maatta et al." *Chemical Physics Letters* (2015).
3. Guo, Xuechao, Alexey B. Nadykto, Yisheng Xu, Qingzhu Zhang, and Jingtian Hu. "Ab intio Investigation of the Thermochemistry and Kinetics of the SO2+ O3−→ SO3−+ O2 Reaction in Aircraft Engines and the Environment." *Entropy* 16, no. 12 (2014): 6300-6312
4. Nadykto, A. B., J. Herb, F. Yu, and Y. Xu, Enhancement due to dimethylamine and large uncertainties in the thermochemistry of amine-enhanced nucleation in the Earth's atmosphere, Chemical Physics Letters, 10.1016/j.cplett.2014.03.036, 2014.
5. Nadykto, A.B., Yu, F. Interaction between common organics and trace nucleation species in the earth's atmosphere: Hydrogen bonding and thermochemistry of pre-nucleation clusters (2013) Mathematical Models of Non-linear Phenomena, Processes and Systems: From Molecular Scale to Planetary Atmosphere PP. 135 – 15

6. Nadykto, A.B., Uvarova, L., Latyshev, A.V. Preface (2013) Mathematical Models of Non-linear Phenomena, Processes and Systems: From Molecular Scale to Planetary Atmosphere PP. xi – xvii
7. Herb, J., Xu, Y., Yu, F., Nadykto, A.B. Large hydrogen-bonded pre-nucleation (HSO4 -)(H 2SO4)m(H2O)kand (HSO 4 -)(NH3)(H2SO4) m(H2O)k clusters in the Earth's atmosphere (2013) Journal of Physical Chemistry A 117 (1) PP. 133 - 152 Cited 5 times. doi: 10.1021/jp3088435
8. Nadykto, A.B., Yu, F. Dipole-charge interactions in nucleating vapours: An overview of recent developments (2013) *Mathematical Models of Non-linear Phenomena, Processes and Systems: From Molecular Scale to Planetary Atmosphere* PP. 123 – 134
9. Nadykto, A.B., Uvarova, L., Latyshev, A.V. Mathematical models of non-linear phenomena, processes and systems: From molecular scale to planetary atmosphere (2013) Mathematical Models of Non-linear Phenomena, Processes and Systems: From Molecular Scale to Planetary Atmosphere PP. 1 – 479
10. Herb, J., Nadykto, A.B., Yu, F.Large ternary hydrogen-bonded pre-nucleation clusters in the Earth's atmosphere (2011) Chemical Physics Letters 518 PP. 7 - 14 doi: 10.1016/j.cplett.2011.10.035
11. Nadykto, Alexey B. Yu, F., Jakovleva, M. V.. Herb, J. and Xu, Y Amines in the Earth's Atmosphere: A Density Functional Theory Study of the Thermochemistry of Pre-Nucleation Clusters, ENTROPY, 13 (2), 554-569
12. Xu, Y., Nadykto, A.B., Yu, F., Jiang, L., Wang, W. Formation and properties of hydrogen-bonded complexes of common organic oxalic acid with atmospheric nucleation precursors (2010) Journal of Molecular Structure: THEOCHEM 951 (1-3) PP. 28 - 33 . doi: 10.1016/j.theochem.2010.04.004
13. Xu, Y., Nadykto, A.B., Yu, F., Herb, J., Wang, W. Interaction between common organic acids and trace nucleation species in the earth's atmosphere (2010) Journal of Physical Chemistry A 114 (1) PP. 387 - 396 Cited 15 times. doi: 10.1021/jp9068575
14. Xu Y., Jiang L., Wang W., Nadykto A.B., Yu F. FORMATION AND PROPERTIES OF HYDROGEN-BONDED COMPLEXES OF COMMON ORGANIC OXALIC ACID WITH ATMOSPHERIC NUCLEATION PRECURSORS Computational and Theoretical Chemistry. 2010. Т. 951. № 1-3. С. 28-33.
15. Nadykto, A. B., F. Yu, and J. Herb, Ammonia in positively charged atmospheric pre-nucleation clusters: A quantum-chemical study and atmospheric implications, Atmos. Chem. Phys., 9, 4031-4038, 2009.
16. Nadykto, A. B., F. Yu, and J. Herb,Theoretical Analysis Of The Gas-Phase Hydration Of Common Atmospheric Pre-Nucleation (HSO4-)(H2O)n and (H3O+)(H2SO4)(H2O)n Cluster Ions, Chemical Physics, 360, 67-73, doi:10.1016/j.chemphys.2009.04.007, 2009.
17. Xu, Y., A. Nadykto, F. Yu, J. Herb, and W. Wang, Interaction between common organic acids and trace nucleation species in the Earth's atmosphere, J. Phys. Chem. A, 10.1021/jp9068575, 2009
18. Nadykto, A. B., F. Yu, and A. Al Natsheh , Anomalously Strong Effect of the Ion Sign on the Thermochemistry of Hydrogen Bonded Aqueous Clusters of Identical Chemical Composition, Int. J. Mol. Sci. 2009, 10(2), 507-517, doi:10.3390/ijms10020507, 2009.
19. Du, H., A. Nadykto, and F. Yu, Quantum-mechanical solution to fundamental problems of classical theory of homogeneous water vapor nucleation, Phys. Rev. E., 79, 021604, 2009.
20. *Nadykto, A. B.*, and F. Yu, Thermochemistry of Nucleating Clusters: A Bridge between the Quantum World and Planetary Atmosphere, in *Thermochemistry: New Research*, Nova Science Publishers, NY, 55-102 (2009)
21. Nadykto, A. B., F. Yu, and J. Herb, Towards understanding the sign preference in binary atmospheric nucleation, Physical Chemistry Chemical Physics, 10, 7073 - 7078, DOI: 10.1039/b807415a, 2008.
22. Nadykto, A. B., F. Yu, and J. Herb, Effect of Ammonia on the Gas-Phase Hydration of Common Atmospheric Ion HSO4- , International Journal of Molecular Sciences, 9(11), 2184-2193, DOI: 10.3390/ijms9112184, 2008.
23. Nadykto, A. B., and F. Yu, Anomalously large difference in dipole moment of isomers with nearly identical thermodynamic stability, Journal of Physical Chemistry, 112, 7222-7226, 2008.

24. A Al Natsheh, F. Yu, K.V. Mikkelsen, and J. Herb, Computational Quantum Chemistry: A New Approach to Atmospheric Nucleation, Advances in Quantum Chemistry, 55, 449-478, 2008 (Review)
25. *Nadykto, A. B.*, F. Yu, and J. Herb, Towards understanding the sign preference in binary atmospheric nucleation, Physical Chemistry Chemical Physics, 2008 DOI:10.1039/B807415A.
26. *Nadykto, A. B.*, and F. Yu, Anomalously large difference in dipole moment of isomers with nearly identical thermodynamic stability, *J. Phys. Chem. A, 112* (31), 7222–7226, 2008
27. *Nadykto, A.B.* and F.Yu, Strong hydrogen bonding between atmospheric nucleation precursors and common organics, *Chemical Physics Letters, 435, 1-3*, 14-18, 2007
28. *Nadykto, A. B.*, A. Al Natsheh, F. Yu, K.V. Mikkelsen, and J.Ruuskanen, Comment, Reply, *Physical Review Letters*, 98**,** 109604, 2007.
29. Nadykto, A., and F. Yu, Thermochemistry of (H2SO4)m(H2O)n(NH3)k: A DFT study, in *Nucleation and Atmospheric Aerosols*, C. D. O'Dowd and P. E. Wagner (eds.), 297-301, Springer 2007.
30. Nadykto, A., and F. Yu, Stabilization of H2SO4-H2O Clusters by Organic Acids, in *Nucleation and Atmospheric Aerosols*, C. D. O'Dowd and P. E. Wagner (eds.), 321-325, Springer 2007.
31. Du., H., A. Nadykto, and F. Yu, Water Homogeneous Nucleation: Model with Quantum-Based Importance of Clustering Thermodynamics, in *Nucleation and Atmospheric Aerosols*, C. D. O'Dowd and P. E. Wagner (eds.), 167-171, Springer 2007
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33. Al Natsheh, A., *A. B. Nadykto*, K. V. Mikkelsen, F. Yu, and J. Ruuskanen, Coexistence of metastable nitric acid dihydrates: A molecular level contribution to understanding the polar stratospheric clouds crystals formation, *Chemical Physics Letters*, 426, 20-25, 2006.
34. *Nadykto, A. B.*, H. Du, and F. Yu, Quantum DFT and DF-DFT study of infrared spectra of sulfuric acid, sulfuric acid monohydrate, formic acid and its cyclic dimer, *Vibrational Spectroscopy*, doi:10.1016/j.vibspec.2007.01.002, 2007.
35. *Nadykto A.B.*, and F. Yu, Simple correction to the classical theory of homogeneous nucleation, *J. Chem. Phys., 122*, 104511 , 2005.
36. *Nadykto, A.B.* and F. Yu, Formation of binary ion clusters from polar vapours: effect of the dipole-charge interaction, *Atmos. Chem. Phys.* 4 (2), 385-389, 2004
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40. *Nadykto A.B.*, J. Mäkelä, F. Yu, M. Kulmala and A. Laaksonen, Comparison of the experimental mobility equivalent diameter for small cluster ions with theoretical particle diameter corrected by effect of vapour polarity, *Chemical Physics Letters*, 382/1-2, 6-11, 2003.
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43. *Nadykto, A.B.* Phase transitions in aerodisperse systems: Transitional condensational growth of non-spherical particles and mobility of ions. In *Mathematical Modeling: Problems, Methods, Applications*, Kluwer Academic/Plenum Publishers, New York, 345-354, 2002.
44. *Nadykto A.B. Condensational growth and evaporation of liquid droplets and ice particles in non-isothermal gas mixtures*. Report Series in *Aerosol Science*, 53, 1-65, 2001 (monograph)
45. *Nadykto A.B.*, E.R. Schukin and L.A.Uvarova, Vaporization and growth of aerosol particles, given internal heat release and radiant heat exchange. In *Mathematical Models of Non-linear Excitations, Dynamics, Transfer and Control in Condensed Systems and Other Media*, Kluwer Academic/Plenum Publishers, New York., 321-334, 1999

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47. Schukin E.R. and *A.B.Nadykto*. Convective (Stefan) vaporaization of large and moderately large particles. In Book *Mathematical Models of Non-Linear Excitations, Dynamics, Transfer and Control in Condensed Systems and Other Media*, Kluwer Academic/Plenum Publishers, New York, 335-350, 1999.
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49. Schukin E.R., *A.B.Nadykto* and Zagayanov V.A. Kinetics of the vaporization and growth of the aerosol particles in the field of internal heat sources in the continuum regime. *VANT, Theoretical and Applied Physics*, 3, 43-52, 1998
50. Schukin E.R. and *A.B.Nadykto.* The effect of the Stefan flux on the evaporation and condensation of the aerosol particles at high temperature gradients in the aerodisperse system. *VANT, Theoretical and Applied Physics*, 2, 57-64, 1998
51. Schukin E.R., *A.B.Nadykto* and Schulinamova Z.L. Heterogeneous combustion of solid particles in a multicomponent gas mixture at low concentration of chemically active components. *VANT, Theoretical and Applied Physics*, 2, 26-30, 1997.