

Andrey G. Kalinichev - Curriculum Vitae

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Education: Ph.D. (Chemical Physics) – Institute of Chemical Physics, Russian Acad. Sci., Moscow, Russia, 1986
B.S., M.S. (Engineering Thermophysics) – Odessa Technological Institute, Odessa, Ukraine, 1977, 1979

Research and Professional Experience:

2010- date, Directeur de Recherche, Laboratoire Subatech (UMR 6457), Institut Mines-Télécom Atlantique, FRANCE
2017- date Chief Research Fellow, International Laboratory for Supercomputer Atomistic Modelling and Multi-Scale Analysis, National Research University Higher School of Economics, Moscow, RUSSIA
2007- 2012, Research Associate Professor, Adjunct Professor, Department of Chemistry, Department of Geological Sciences, Michigan State University, USA
2000-2007, Research Associate Professor, Senior Research Scientist, Department of Geology, University of Illinois at Urbana-Champaign, USA
1998-2000, Visiting Senior Research Scientist / Visiting Assistant Professor, Department of Geology, Department of Chemistry, University of Illinois at Urbana-Champaign, USA
1994-2000, Head, Physical Research Laboratory, Institute of Experimental Mineralogy, Russian Academy of Sciences, Chernogolovka, Moscow Region, RUSSIA
1992-1994, Visiting Research Associate, Department of Geology, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, USA
1991-1994, Head, Computer Modeling Research Group, Inst. of Experimental Mineralogy, Russian Academy of Sciences, Chernogolovka, Moscow Region, RUSSIA
1989-1991, Alexander von Humboldt Research Fellow, Research Group of Physical Chemistry, Max-Planck-Institut für Chemie (Otto-Hahn-Institut), Mainz, GERMANY
1979-1989, Research Associate, Senior Research Associate, Laboratory of Hydrothermal Processes, Institute of Experimental Mineralogy, Russian Academy of Sciences, Chernogolovka, RUSSIA

Awards and Distinctions:

2015 Special medal of the Russian Society for Supercritical Fluids for pioneering contributions to the research in the area of supercritical fluid science and technology in Russia.
2013 George W. Brindley Lecture Award of the Clay Minerals Society for 2013.
2007-2009 Undergraduate student travel award for the International School of Earth Sciences at the Department of Geology, Moscow State University, Russia, is named in honor of A. G. Kalinichev
1997 Research Award in Earth, Environmental, and Energy Sciences from INTAS, European Union
1993 Shared University Research Award from the IBM Corp., University of Illinois, Urbana, IL, USA
1989-1991 Alexander von Humboldt Research Fellowship, Alexander von Humboldt Foundation, GERMANY

Recent Professional Activities:

- Vice-President – *The Clay Minerals Society* (2018 - present)
- Guest Editor – *Minerals*, Special Issue “Molecular Simulation of Mineral-Solution Interfaces” (2016-2018)
- Guest Editor – *Journal of Molecular Liquids*, Special Issue “Supercritical fluids: Theory and applications” (2016-2017)
- Co-Editor – The Geological Society of London Special Publication SP400: “Clays in Natural and Engineered Barriers for Radioactive Waste Confinement” (2013-2014)
- Associate Editor – *Supercritical Fluids – Theory and Praxis (Russia)* (2019 - present)
- Associate Editor – *Clays and Clay Minerals* (2014 - present)
- Organizer and Co-Chairman – Special Session “Computational modeling of clay minerals”, 16th Intern. Clay Conf., Lecturer – AIPEA School for Young Scientists “Computational modeling in clay mineralogy”, July 15-21, 2017, Granada, Spain
- Organizer and Co-Chairman – Special Session “(Bio-)geochemistry of layered materials: From molecular-scale structure and reactivity to field-scale applications” Goldschmidt-2016 Conf., June 26 - July 1, 2016, Yokohama, Japan
- Organizer and Co-Chairman – Special Session “Molecular simulation of clay minerals and reactions”, 51th Annual Meeting of the Clay Minerals Society, May 17-21 2014, College Station, TX, USA
- Organizer and Co-Chairman – Special Session “Modeling the interface: mineralogy, environment and energy applications”, 247th American Chemical Society National Meeting, March 16-20 2014, Dallas, TX, USA
- Member of the Scientific Committee – 5th International Meeting “Clays in Natural & Engineered Barriers for Radioactive Waste Confinement”, Montpellier, France (2011-2012)
- Manuscript reviewer – over 30 reviews annually for 20+ professional research journals on molecular modeling of materials, material-water interfaces and related topics (among top 20% reviewers for the *J. Phys. Chem.*)
- Proposal reviewer and panel review member – over 70 research proposals reviewed in the last 10 years for the US Department of Energy Geosciences and Nuclear Energy Programs; NSF Earth Sciences and Chemistry Programs; King Abdulaziz City for Science & Technology (Saudi Arabia); Ministry for Science and Education (Russia)
- Member – American Chemical Society; Clay Minerals Society; Geochemical Society; European Association of Geochemistry; European Molecular Liquids Group

Publications: Author/co-author of over 130 peer-reviewed articles on the topics of molecular computer simulations of aqueous fluids and mineral-fluid interfaces: <http://www.researcherid.com/rid/B-4519-2008>.

Most Recent Publications:

- 1) M. Pouvreau, J.A. Greathouse, R.T. Cygan, A.G. Kalinichev (2019) Structure of hydrated kaolinite edge surfaces: DFT results and further development of the ClayFF classical force field with metal-O-H angle bending terms. *J. Phys. Chem. C*, **123**, 11628-11638.
- 2) N. Loganathan, G. M. Bowers, B.F. Ngouana-Wakou, A. G. Kalinichev, R. J. Kirkpatrick, A. O. Yazaydin (2019) Understanding methane/carbon dioxide partitioning in clay nano- and meso-pores with constant reservoir composition molecular dynamics modeling, *Phys. Chem. - Chem. Phys.*, **21**, 6917-6924.
- 3) N. Loganathan, G. M. Bowers, A. O. Yazaydin, A. G. Kalinichev, R. J. Kirkpatrick (2018) Competitive adsorption of H₂O and CO₂ in 2-dimensional nano-confinement: GCMD simulations of Cs- and Ca-hectorite. *J. Phys. Chem. C*, **122**, 23460-23469.
- 4) N. Loganathan, G.M. Bowers, A.O. Yazaydin, H.T. Schaef, J. Loring, A.G. Kalinichev, R.J. Kirkpatrick (2018) Clay swelling in dry supercritical carbon dioxide: Effects of interlayer cations on the structure, dynamics, and energetics of CO₂ intercalation probed by XRD, NMR and GCMD simulations. *J. Phys. Chem. C*, **122**, 4391-4402.
- 5) R.K. Mishra, A.K. Mohamed, D. Geissbühler, H. Manzano, T. Jamil, R. Shahsavari, A.G.Kalinichev, S. Galmarini, L. Tao, H. Heinz, R. Pellenq, A.C.T. van Duin, S.C. Parker, R.J. Flatt, P. Bowen (2017) CemFF: A force field database for cementitious materials- validations, applications and opportunities. *Cem. Concr. Research*, **102**, 68-89.
- 6) N.Loganathan, A.O.Yazaydin, G.M.Bowers, A.G.Kalinichev, R.J.Kirkpatrick (2017) Molecular dynamics study of CO₂ and H₂O intercalation in smectite clays: Effect of temperature and pressure on interlayer structure and dynamics in hectorite. *J. Phys. Chem. C*, **121**, 24527-24540.
- 7) A.G. Kalinichev (2017) Universality of hydrogen bond distributions in liquid and supercritical water. *Journal of Molecular Liquids*, **241**, 1038-1043.
- 8) M. Pouvreau, J.A. Greathouse, R.T. Cygan, A.G. Kalinichev (2017) Structure of hydrated gibbsite and brucite edge surfaces: DFT results and further development of the ClayFF classical force field with metal-O-H angle bending terms. *J. Phys. Chem. C*, **121**, 14757-14771.
- 9) I. Androniuk, C. Landesman, P. Henocq, A.G. Kalinichev (2017) Adsorption of gluconate and uranyl on C-S-H phases: combination of wet chemistry experiments and molecular dynamics simulations. *Physics and Chemistry of the Earth, Parts A/B/C*, **99**, 194-203.
- 10) N.Loganathan, A.G.Kalinichev (2017) Quantifying the mechanisms of site-specific ion exchange at an inhomogeneously charged surface: Case of Cs⁺/K⁺ on hydrated muscovite mica. *J. Phys. Chem. C*, **121**, 7829-7836.

Most Highly Cited Publications (current h-index: 37)

- 1) R.T.Cygan, J.-J.Liang, A.G.Kalinichev (2004) Molecular models of hydroxide, oxyhydroxide, and clay phases and the development of a general force field. *Journal of Physical Chemistry B*, **108**, 1255-1266 (982 citations).
- 2) J.Wang, A.G.Kalinichev, R.J.Kirkpatrick (2006) Effects of substrate structure and composition on the structure, dynamics and energetics of water on mineral surfaces: a molecular dynamics modeling *Geochimica et Cosmochimica Acta*, **70**, 562-582 (181 citations).
- 3) Yu.E.Gorbaty, A.G.Kalinichev (1995) Hydrogen bonding in supercritical water. 1. Experimental results. *Journal of Physical Chemistry*, **99**, 5336-5340 (161 citations).
- 4) A.G.Kalinichev, J.D.Bass (1997) Hydrogen bonding in supercritical water. 2. Computer simulations. *Journal of Physical Chemistry A*, **101**, 9720-9727 (160 citations).
- 5) A.G.Kalinichev, R.J.Kirkpatrick (2002) Molecular dynamics modeling of chloride binding to the surfaces of Ca-hydroxide, hydrated Ca-aluminate and Ca-silicate phases. *Chemistry of Materials*, **14**, 3539-3549 (158 citations).
- 6) J.Wang, A.G.Kalinichev, R.J.Kirkpatrick, R.T.Cygan (2005) Structure, energetics, and dynamics of water adsorbed on the muscovite (001) surface: A molecular dynamics simulation. *J. Phys. Chem. B*, **109**, 15893-15905 (155 cit.).
- 7) R.T.Cygan, J.A.Greathouse, H.Heinz, A.G.Kalinichev (2009) Molecular models and simulations of layered materials. *Journal of Materials Chemistry*, **19**, 2470-2481 (151 citations).
- 8) J.Wang, A.G.Kalinichev, R.J.Kirkpatrick, X.Hou (2001) Molecular modeling of the structure and energetics of hydrotalcite hydration. *Chemistry of Materials*, **13**, 145-150 (120 citations).
- 9) A.G.Kalinichev, J.Wang, R.J.Kirkpatrick (2007) Molecular dynamics modeling of the structure, dynamics and energetics of mineral-water interfaces: Application to cement materials. *Cement and Concrete Research*, **37**, 337-347 (117 citations).
- 10) A.G.Kalinichev (2001) Molecular simulations of liquid and supercritical water: Thermodynamics, structure, and hydrogen bonding. *Reviews in Mineralogy and Geochemistry*, **42**, 83-129 (97 citations).

Collaborators in the past 5 years:

R.J.Kirkpatrick, G.M.Bowers, N.Loganathan, A.Ö.Yazaydin, C.P.Morrow, (Michigan State Univ.)
R.T.Cygan, J.A.Greathouse (Sandia National Labs) / P.Henocq (ANDRA, France) / A.I.Kolesnikov (SNS, ORNL)
H.Heinz (University of Colorado, Boulder) / P.Kumar (Indian Inst. of Technology) / C.Tournassat (BRGM, France)
J.Wang (Louisiana State Univ.) / B.Grambow, C.Landesman, G.Montavon, B.F.Ngouana-Wakou (Subatech, IMT-A)
M.Szczerba, A. Derkowski, J. Środoń (Institute of Geological Sciences, Polish Academy of Sciences, Poland)
G.E.Norman, V.V.Stegailov (NRU Higher School of Economics, Moscow, Russia) / X.Liu, (Nanjing Univ., P.R.China)
A.Striolo (UCL, London) / M.Lisal (ICPF, Prague) / I.Economou (Texas A&M Univ. at Qatar, Doha)