

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 National University of Technology, Odessa, Ukraine, 1974-1979

Research and Professional Experience:

2010- date, Directeur de Recherche, Laboratoire Subatech (UMR 6457), Institut Mines-Télécom Atlantique, FRANCE
2017- 2022 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:

- Editor in Chief – *Minerals*, Section “Clays and Engineered Mineral Materials” (2021 -present)
- Associate Editor – *Discover Minerals* (2023 - present)
- Associate Editor – *Frontiers in Nuclear Engineering* (2022 - present)
- President – *The Clay Minerals Society* (2019 - 2020)
- Associate Editor – *Supercritical Fluids – Theory and Praxis (Russia)* (2018 - 2022)
- Guest Editor – *Journal of Molecular Liquids*, Special Issue “Supercritical fluids: Theory and applications” (2016-2017)
- Associate Editor – *Clays and Clay Minerals* (2014 - present)
- Organizer and Chairman – Thematic Session “*Multiscale computational modeling of clay-related minerals and their fluid interfaces*”, 17th International Clay Conference, (2020-2022), Istanbul, Turkey
- Co-Organizer and Co-Chairman, Special Session “*Experimental and Computational Approaches to Molecular-Scale Understanding of Mineral-Fluid Interactions (Session in memory of R. James Kirkpatrick)*”, American Chemical Society - Fall National Meeting, August 22-26, 2021, Atlanta, GA, USA
- Co-Organizer and Co-Chairman, Special Session 6h: “*Coupled Chemical and Physical Processes in Nano- and Meso-Porous Rocks: Linking Experiments and Computational Modeling over Multiple Scales*”, Goldschmidt-2021 Conference, Lyon, France, July 4-9, 2021
- Member of the Scientific Committee, *XVI Colloque Annuel Groupe Français des Argiles*, 2019-2021, Nantes, France
- 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 150 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) A.D.Krot, I.E.Vlasova, E.V.Tararushkin, A.G.Kalinichev (2024) Atomistic computer simulations of uranyl adsorption on hydrated illite and smectite surfaces. *Minerals*, **14**, 109.
- 2) E.V.Tararushkin, G.S.Smironov, A.G.Kalinichev (2023) Structure and properties of water in a new model of the 10 Å phase: Classical and ab initio atomistic computational modeling. *Minerals*, **13**, 1018.
- 3) E.V.Tararushkin, V.V.Pisarev, A.G.Kalinichev (2023) Interaction of nitrite ions with hydrated portlandite surfaces: Atomistic computer simulation study. *Materials*, **16**, 5026.
- 4) E.V.Tararushkin, V.V.Pisarev, A.G.Kalinichev (2023) Equation of state, compressibility, and vibrational properties of brucite over wide pressure and temperature ranges: Atomistic computer simulations with the modified ClayFF classical force field. *Minerals*, **13**, 408.
- 5) V.V.Pisarev, A.G.Kalinichev (2022) Couette flow of pentane in clay nanopores: Molecular dynamics simulation. *Journal of Molecular Liquids*, **366**, 120290.
- 6) M.A.Logunov, A.G.Kalinichev, V.V.Pisarev (2022) Structure of hydrocarbon fluid and Couette flows in slit pores with pyrophyllite walls. *Polymer Science, Series A*, **64**, 908-917.
- 7) X.Liu, C.Tournassat, S.Grangéon, A.G.Kalinichev, Y.Takahashi, M. Marques Fernandes (2022) Molecular-level understanding of metal ion retention in clay-rich materials. *Nature Reviews Earth & Environment*, **3**, 461-476.
- 8) E.V.Tararushkin, V.V.Pisarev, A.G.Kalinichev (2022) Atomistic simulations of ettringite and its aqueous interfaces: Structure and properties revisited with the modified ClayFF force field. *Cem. Concr. Research*, **156**, 106759.
- 9) K.Damodaran, J.-M. Delaye, A.G.Kalinichev, S.Gin (2022) Deciphering the non-linear impact of Al on chemical durability of silicate glass. *Acta Materialia*, **225**, 117478.
- 10) K.B.Yu, G.M.Bowers, N.Loganathan, A.G.Kalinichev, A.O.Yazaydin (2021) Diffusion behavior of methane in 3D kerogen models. *Energy & Fuels*, **35**, 16515-16526.
- 11) R.T. Cygan, J.A. Greathouse, A.G. Kalinichev (2021) Advances in Clayff molecular simulation of layered and nanoporous materials and their aqueous interfaces. *J. Phys. Chem. C*, **125**, 17573-17589
- 12) A.G. Kalinichev (2021) Atomistic modeling of clays and related nanoporous materials with ClayFF force field. In: Sainz-Díaz, C.I. (Ed.), *Computational Modeling in Clay Mineralogy. AIPEA Educational Ser.*, **3**, 17-52.
- 13) D.I.Grekov, A.G.Kalinichev, T.Suzuki-Muresan, P.Pré, B.Grambow (2021) Direct experimental evidence of the effects of clay particles' basal-to-lateral surface ratio on CH₄/CO₂ adsorption. *J.Phys. Chem.C*, **125**, 11499-11507.

Most Highly Cited Publications (current h-index: 44)

- 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 (2,010 citations).
- 2) 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 (240 citations).
- 3) 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 (236 citations).
- 4) 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 (227 citations).
- 5) 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 (207 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 (200 cit.).
- 7) A.G.Kalinichev, J.D.Bass (1997) Hydrogen bonding in supercritical water. 2. Computer simulations. *Journal of Physical Chemistry A*, **101**, 9720-9727 (188 citations).
- 8) Yu.E.Gorbaty, A.G.Kalinichev (1995) Hydrogen bonding in supercritical water. 1. Experimental results. *Journal of Physical Chemistry*, **99**, 5336-5340 (187 citations).
- 9) W.Y.Ahn, A.G.Kalinichev, M.M.Clark (2008) Effects of background cations on the fouling of polyethersulfone membranes by natural organic matter: Experimental and molecular modeling study. *J. Membr. Sci.*, **309**, 128-140 (155 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 (121 citations).

Collaborators in the past 5 years:

B.Grambow, C.Landesman, G.Montavon, D.Grekov, S.Mutisya (Subatech, IMT-Atlantique, France) / P.Henocq (ANDRA, France) / J.-M.Delaye, S.Gin (CEA-Marcoule, France) / C.Tournassat (BRGM, France) / R.T.Cygan, J.A.Greathouse (Sandia National Labs, US) / R.J.Kirkpatrick, G.M.Bowers, N.Loganathan (Michigan State Univ., US) / M.Szczerba, A. Derkowski, J. Środoń (Institute of Geological Sciences, Polish Academy of Sciences, Poland) / A.N.Ay, B.Zumreoglu-Karan (Hacettepe University, Ankara, Turkey) / X.Liu, (Nanjing Univ., P.R.China) / E.V.Tararushkin, V.V.Pisarev, G.S.Smironov (HSE University, Moscow, Russia) / A.D.Krot, I.E.Vlasova (Moscow State Univ., Russia)