

**Andrey G. Kalinichev**  
*Curriculum Vitae*

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

Professional History:

2007- date, Research Associate Professor, Department of Chemistry, Michigan State University  
2000-2007, Research Associate Professor, Senior Research Scientist, Department of Geology, University of Illinois at Urbana-Champaign  
1998-2000, Visiting Senior Research Scientist / Visiting Assistant Professor, Department of Geology, Department of Chemistry, University of Illinois at Urbana-Champaign  
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  
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  
1984-1989, Research Associate, Senior Research Associate, Laboratory of Hydrothermal Processes, Inst. of Experimental Mineralogy, Russian Academy of Sciences, Chernogolovka, Russia  
1979-1984, Graduate Research Associate, Laboratory of Hydrothermal Systems, Inst. of Experimental Mineralogy, Russian Academy of Sciences, Chernogolovka, Russia

Honors and Awards:

2007, 2008 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 the International Association for the Promotion of Cooperation with Scientists from the Former Soviet Union (INTAS)  
1993 Shared University Research (SUR) Award from the IBM Corp., UIUC  
1989-1991 Alexander von Humboldt Research Fellowship, Alexander von Humboldt Foundation, Germany

Current Research Interests:

- Molecular modeling of the structure and dynamics of aqueous solutions at interfaces and in nano-confinement with inorganic and organic materials, clays, cement phases, polymer membranes, etc.
- Structure, dynamics, and energetics of hydrogen bonding in aqueous systems over wide ranges of thermodynamic conditions
- Supercritical fluids and their technological applications
- Environmental materials chemistry
- Inelastic and quasi-elastic neutron spectroscopy of the hydrous materials

***Publications:*** Author/co-author of over 80 refereed articles and book chapters, mostly on the topics of molecular computer simulations of aqueous solutions and mineral-solution interfaces. The full list of publications and most PDF reprints are available at: <http://www.msu.edu/~kalinich/publications.html>.

***Most Recent Publications:***

- 1) 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. [\*Journal of Membrane Science\*, \*\*309\*\*, 128-140.](#)
- 2) P.Kumar, A.G.Kalinichev, R.J.Kirkpatrick (2007b) Molecular dynamics simulation of the energetics and structure of layered double hydroxides intercalated with carboxylic acids. [\*Journal of Physical Chemistry C\*, \*\*111\*\*, 13517-13523.](#)
- 3) A.G.Kalinichev, R.J.Kirkpatrick (2007) Molecular dynamics simulation of cationic complexation with natural organic matter. [\*European Journal of Soil Science\*, \*\*58\*\*, 909-917.](#)
- 4) I.S.Ufimtsev, A.G.Kalinichev, T.J.Martinez, R.J.Kirkpatrick (2007) A charged ring model for classical OH(aq) simulations. [\*Chemical Physics Letters\*, \*\*442\*\*, 128-133.](#)
- 5) P.Kumar, A.G.Kalinichev, R.J.Kirkpatrick (2007a) Dissociation of carbonic acid: Gas phase energetics and mechanism from *ab initio* metadynamics simulations. [\*J. Chem.Phys.\*, \*\*126\*\*, 204315-1-7.](#)
- 6) 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.](#)
- 7) J.-P. Korb, P.J. McDonald, L. Monteilhet, A.G. Kalinichev, R.J. Kirkpatrick (2007) Comparison of proton field-cycling relaxometry and molecular dynamics simulations for proton–water surface dynamics in cement-based materials. [\*Cement and Concrete Research\*, \*\*37\*\*, 348-350.](#)

***Most Highly Cited Publications (current h-index: 21)***

- 1) Yu.E.Gorbaty, A.G.Kalinichev (1995) Hydrogen bonding in supercritical water. 1. Experimental results. [\*Journal of Physical Chemistry\*, \*\*99\*\*, 5336-5340](#) (113 citations).
- 2) A.G.Kalinichev, J.D.Bass (1997) Hydrogen bonding in supercritical water. 2. Computer simulations. [\*Journal of Physical Chemistry A\*, \*\*101\*\*, 9720-9727](#) (96 citations).
- 3) 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. [\*J. Phys. Chem. B\*, \*\*108\*\*, 1255-1266](#) (84 cit.).
- 4) A.G.Kalinichev, J.D.Bass (1994) Hydrogen bonding in supercritical water: a Monte Carlo simulation. [\*Chemical Physics Letters\*, \*\*231\*\*, 301-307](#) (68 citations).
- 5) 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](#) (55 citations).
- 6) 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](#) (51 citations).
- 7) A.G.Kalinichev, R.J.Kirkpatrick, R.T.Cygan (2000) Molecular modeling of the structure and dynamics of the interlayer and surface species of mixed-metal layered hydroxides: Chloride and water in hydrocalumite (Friedel's salt). [\*American Mineralogist\*, \*\*85\*\*, 1046-1052](#) (41 citations).
- 8) A.G.Kalinichev (2001) Molecular simulations of liquid and supercritical water: Thermodynamics, structure, and hydrogen bonding. [\*Reviews in Mineralogy and Geochemistry\*, \*\*42\*\*, 83-129](#) (38 citations).

***Collaborators in past 48 months:***

R.J.Kirkpatrick, G.Bowers (Michigan State University) / R.T.Cygan (Sandia National Laboratories)  
W.-Y.Ahn, M.M.Clark, X.Hou, T.J.Martinez, L.J.Struble I.S.Ufimtsev, X.Xu (University of Illinois)  
G.V.Bondarenko, Y.E.Gorbaty, A.V.Okhulkov (Russian Acad. of Sciences) / J.J.Liang (Accelrys, Inc.)  
J.Wang (University of Michigan) / P.Kumar (Indian Institute of Technology) / J.Amonette (PNNL)  
A.I.Kolesnikov (SNS, ORNL) / A.Faraone, T.J.Udovic (NIST) / N. R. de Souza (FZ Jülich, Germany)  
U.Deiters (University at Cologne, Germany) / J.-P.Korb (Ecole Polytechnique, Palaiseau, France)  
M.X.Reinholdt (Université Laval, Cité Universitaire Québec, Canada)