

## Jianwei Wang

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### EDUCATION:

#### **Ph.D. in Geochemistry, University of Illinois at Urbana-Champaign, Illinois, USA. 10/2004.**

Dissertation: Molecular structure, energetics, and dynamics of water at mineral interlayers and surfaces in environmental and geochemical systems. Advisor: Professor R. James Kirkpatrick.

### RESEARCH EXPERIENCE

#### **10/2006-present: Research Fellow. University of Michigan, Ann Arbor, Michigan, USA.**

High-performance computer modeling and simulations: Applications of quantum chemistry and molecular dynamics in Earth materials and geochemistry.

- Gas hydrates, hydrogen clathrate hydrate for hydrogen storage.
  - Order-disorder and defect in complex oxides and nuclear waste forms.
  - Chemistry of water-vapor interface.
  - Nanoparticles in the environment.
  - Interaction between biomaterials and mineral surfaces, biominerals, biomineralization.
  - Material's phase behaviors (defect, phase transition, melting) at high pressure and irradiation.
- These researches are highly facilitated by supercomputer centers including TeraGrid (NCSA, NICS) and NERSC.

#### **10/2004-09/2006: Postdoctoral Researcher. University of California, California, USA.**

Large scale molecular simulations by first principles calculations and molecular dynamics simulations.

- Chemical reactivity and hydration of hematite.
- Thermodynamics and kinetics of water exchange reaction at aqueous ions, nanoparticles, and mineral surfaces.
- Stability and thermodynamics of mineral nanoparticles

#### **07/1998-10/2004: Research assistant and fellowship. University of Illinois, Illinois, USA.**

Interactions of water with mineral interlayer and surfaces by computational molecular dynamics simulations.

- Molecular structure, vibrational spectroscopy, and hydration of layered double hydroxides.
- Molecular structure of confined water.
- Hydrogen bonding network, structural ordering, diffusive dynamics, energetics of hydration of interfacial water at mineral surfaces.

### FIELDS OF SPECIALIZATION

**Physical sciences and geosciences:** Thermodynamics, statistical mechanics, physical chemistry, surface and colloids, mineral surfaces. Mineralogy/mineral physics, structure mineralogy, low

temperature environmental geochemistry, mineral-water interaction, interfacial geochemistry, mineral surface reactivity, aqueous geochemistry.

**Modeling and simulations in computational mineralogy and Earth materials sciences:** Atomistic-scale modeling, empirical potential molecular dynamics, and first-principles simulations. Frequent used programs: CERIU2, MATERIAL STUDIO, GAUSSIAN, VASP, DL\_POLY, GROMACS, LAMMPS, and SIESTA. Daily access to high-performance supercomputers of both shared and distributed memory machines.

## MEMBERSHIP IN PROFESSIONAL SOCIETIES

American Chemical Society (2005-), American Geophysical Union (2002-), Clay Minerals Society (2000-), Geochemical Society (2001-), Mineralogical Society of America (1999-).

## TOP FIVE CITED PAPERS (current h-index: 8, total citations: 240)

1. J. Wang, A.G. Kalinichev, R.J. Kirkpatrick, and X. Hou. (2001) Molecular modeling of the structure and energetics of hydrotalcite hydration. *Chemistry of Materials*, 13, 145-150. **(62 citations)**
2. J. Wang, A.G. Kalinichev, J.E. Amonette, and R.J. Kirkpatrick. (2003) Interlayer structure and dynamics of Cl-hydrotalcite: Far infrared spectroscopy and molecular dynamics modeling. *American Mineralogist*, 88, 398-409. **(33 citations)**
3. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. (2006) Effects of substrate structure and composition on the structure, dynamics, and energetics of water at mineral surfaces: A molecular dynamics modeling study. *Geochimica et Cosmochimica Acta*. 70, 562-582. **(32 citations)**
4. J. Wang, A. G. Kalinichev, and R.J. Kirkpatrick. (2004) Molecular modeling of water structure in nano-pores between brucite (001) surfaces. *Geochimica et Cosmochimica Acta.*, 68(16), 3351-3365. **(28 citations)**
5. J. Wang, A.G. Kalinichev, R.J. Kirkpatrick, and R.T. Cygan. (2005) Structure, energetics, and dynamics of water adsorbed on the muscovite (001) surface: a molecular dynamics simulation. *Journal of Physical Chemistry B*. 109, 15893-15905. **(25 citations)**

## PUBLICATIONS

1. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick (2009) Asymmetric hydrogen bonding and orientational ordering of water at hydrophobic and hydrophilic surfaces: a comparison of water/vapor, water/talc, and water/mica interfaces. *Journal of Physical Chemistry C*, 113, 11077-11085.
2. J. Wang and Udo Becker (2009) Structure and carbonate orientation of vaterite (CaCO<sub>3</sub>). *American Mineralogist*, 94, 380-386.
3. F. Zhang, M.K. Lang, J. Wang, U. Becker, and R.C. Ewing (2008) Structural phase transitions of cubic Gd<sub>2</sub>O<sub>3</sub> at high pressures. *Physical Review B*, 78, 064114.
4. F. Zhang, J. Wang, J. Lian, M.K. Lang, U. Becker, and R.C. Ewing (2008) Phase stability and pressure dependence of defect formation in Gd<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> and Gd<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> pyrochlores. *Physical Review Letters*, 100, 045503.
5. F. Zhang, J. Wang, U. Becker, J. Lian, J. Hu, S. Saxena, and R.C. Ewing (2007) Pressure-Induced Splitting and Buckling of Cu-O Chains in the Low-Dimensional Structure of SrCuO<sub>2</sub>. *Journal of the American Chemical Society*, 129, 13923-13926.
6. J. Wang, J.R. Rustad, and William H. Casey (2007) Water-exchange reactions on aluminous clays and minerals. *Inorganic Chemistry*, 46, 2962-2964.

7. A.G. Kalinichev, J. Wang, and 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.
8. J. Wang and J.R. Rustad (2006) A simple model for the effect of hydration on the distribution of ferrous iron at reduced hematite (012) surfaces. *Geochimica et Cosmochimica Acta*, 70, 5285-5292.
9. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. (2006) Effects of substrate structure and composition on the structure, dynamics, and energetics of water at mineral surfaces: A molecular dynamics modeling study. *Geochimica et Cosmochimica Acta*. 70, 562-582.
10. J. Wang, A.G. Kalinichev, R.J. Kirkpatrick, and R.T. Cygan. (2005) Structure, energetics, and dynamics of water adsorbed on the muscovite (001) surface: a molecular dynamics simulation. *Journal of Physical Chemistry B*. 109, 15893-15905.
11. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. (2005) Structure and decompression melting of a novel, high-pressure nanoconfined 2-d ice. *Journal of Physical Chemistry B*. 109, 14308-14313.
12. R.J. Kirkpatrick, A.G. Kalinichev, and J. Wang, (2005) Molecular Dynamics Modeling of Hydrated Mineral Interlayers and Surfaces: Structure and Dynamics. *Mineralogical Magazine*, 69(3), 289-308.
13. J. Wang, A. G. Kalinichev, and R.J. Kirkpatrick. (2004) Molecular modeling of water structure in nano-pores between brucite (001) surfaces. *Geochimica et Cosmochimica Acta.*, 68(16), 3351-3365.
14. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. (2004) Molecular modeling of the 10-Å phase at subduction zone conditions. *Earth and Planetary Sciences Letters*, 222, 517-527.
15. Kirkpatrick R.J., Kalinichev A.G., Wang J., Hou X., and Amonette J.E. (2004) Molecular modeling of the vibrational spectra of interlayer and surface species of layered double hydroxides. In: *The Application of Vibrational Spectroscopy to Clay Minerals and Layered Double Hydroxides*, CMS Workshop Lectures, vol. 13, J. Theo Kloprogge, ed., The Clay Minerals Society, Aurora, CO, pp.239-285.
16. J. Wang, A.G. Kalinichev, J.E. Amonette, and R.J. Kirkpatrick. (2003) Interlayer structure and dynamics of Cl-hydroxalite: Far infrared spectroscopy and molecular dynamics modeling. *American Mineralogist*, 88, 398-409.
17. A.G. Kalinichev, J. Wang, R.J. Kirkpatrick, and R.T. Cygan. (2001) Molecular dynamics simulation of layered double hydroxides. *AIChE Symposium Series*, 325, 251-255.
18. J. Wang, A.G. Kalinichev, R.J. Kirkpatrick, and X. Hou. (2001) Molecular modeling of the structure and energetics of hydroxalite hydration. *Chemistry of Materials*, 13, 145-150.

#### CONFERENCE ABSTRACTS:

1. J. Wang, F. Zhang, J. Lian, R.C. Ewing, and U. Becker. Energetics of defect formation in pyrochlore,  $Gd(Ti/Zr)_2O_7$ , at high pressure. The 2008 Materials Research Society Fall Meeting, Boston, MA, December 1-5, 2008.
2. U. Becker, S. Biswas, and J. Wang. Dynamic simulations of polypeptide templates to promote Ca-carbonate nuclei. 2008 AGU Fall Meeting, San Francisco, California. December 15-19, 2008
3. U. Becker, M. Reich, S. Utsunomiya, J. Wang, S. Kesler, L. Wang, R.C. Ewing. Nanoparticle-host interactions in natural systems. 2008 AGU Fall Meeting, San Francisco, California. December 10-14, 2007.
4. U. Becker, M. Reich, S. Utsunomiya, R.C. Ewing, L. Wang, J. Wang. The fate of. 2007 AGU Joint Assembly Acapulco, Mexico, May 22-25, 2007.
5. J.R. Rustad, J. Wang, and W.H. Casey. Site-specific, size-dependent reactivity of Al-oxide nanoparticle surfaces 17th Annual V M Goldschmidt Conference, AUG, 2007 Cologne, GERMANY. August 19 - 24, 2007

6. J.R. Rustad, W.H. Casey, and J. Wang. Site-specific, size-dependent reactivity of Al-oxide nanoparticle surfaces. Computational and Numerical Geosciences, the thirteenth in a series of Geosciences Research Program Symposia (DOE). Gaithersburg, MD, USA. May 3-4, 2007.
7. J. Wang and J.R. Rustad. Effect of hydration on the ferrous ion distribution at reduced hematite (012) surface. American Chemical Society 232nd National Meeting & Exposition, San Francisco, CA, USA. September 10-14, 2006.
8. J. Wang, J.R. Rustad, and W.H. Casey. Energetics and mechanism of water exchange at aqueous Al-bearing ions and nanoparticles. American Chemical Society 232nd National Meeting & Exposition, San Francisco, CA, USA. September 10-14, 2006.
9. A.G. Kalinichev, J. Wang, and R.J. Kirkpatrick. Molecular dynamics of mineral-water interfaces: Structure, dynamics, energetics and hydrogen bonding. American Chemical Society 232nd National Meeting & Exposition, San Francisco, CA, USA. September 10-14, 2006.
10. J.R. Rustad, J. Wang. Distribution of reduced iron at ferric oxide surfaces. 16th Annual V M Goldschmidt Conference, AUG-SEP, 2006 Melbourne, AUSTRALIA. August 27 - September 01, 2006.
11. A.G. Kalinichev, J. Wang, and R.J. Kirkpatrick. Molecular ordering, structure, and dynamics of water at mineral surfaces: MD computer simulation. 2006 Materials Research Society Spring Meeting, San Francisco, California, USA, April 17-21, 2006.
12. J. Wang and J.R. Rustad. Hydration effect on charge distribution of reduced hematite (012) surface. The 15th Goldschmidt Conference of Geochemical Society, Moscow, Idaho, USA, 20-25 May, 2005.
13. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. Molecular Dynamics Modeling of the Structure of Water on Solid Surfaces 107th Annual Meeting & Exposition of The American Ceramic Society, Baltimore, Maryland, USA, April 10-13, 2005.
14. R.J. Kirkpatrick, J. Wang, and A.G. Kalinichev. Molecular modeling of the 10Å phase at subduction zone conditions. 2004 AGU Fall Meeting, San Francisco, California. December 13-17, 2004.
15. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. Structure and decompression melting of a novel 2-D high pressure ice phase formed in nano-confinement between two talc surfaces. 2004 AGU Fall Meeting, San Francisco, California. December 13-17, 2004.
16. A.G. Kalinichev, R.J. Kirkpatrick, and J. Wang. Hydrogen bonding, hydration of species, ion pairing and clusterization in H<sub>2</sub>O-NaCl-CaCl<sub>2</sub>-CO<sub>2</sub>-NaHCO<sub>3</sub>-Na<sub>2</sub>CO<sub>3</sub> fluids: Molecular dynamics simulation of the effects of temperature, pressure and composition. 2004 AGU Fall Meeting, San Francisco, California. December 13-17, 2004.
17. R.J. Kirkpatrick, A.G. Kalinichev, and J. Wang. Molecular Dynamics Modeling of Hydrated Mineral Interlayers and Surfaces: Structure and Dynamics. Proton-mediated interactions in minerals sponsored by the Mineralogical Society of Great Britain & Ireland. University of Manchester, UK. September 13-14, 2004.
18. R.J. Kirkpatrick, A.G. Kalinichev, and J. Wang. Molecular Dynamics Modeling of Structure and Dynamics in Cement Materials. Conference to Celebrate the Contribution of HFW (Hal) TAYLOR to Cement and Concrete Science. Les Diablerets, Switzerland. June 20 – 23, 2004.
19. R.T. Cygan, J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. Molecular models of the external surfaces of kaolinite and the dynamics of the clay-water interface. 14th Annual V. M. Goldschmidt Conference, Copenhagen, Denmark, June 5 -11, 2004.
20. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. Molecular modeling of water on the muscovite (001) surface. 227th ACS National Meeting, Anaheim, California, March 28 - April 1, 2004.
21. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. The structure of water in nano-confinement between two talc (001) surfaces. 227th ACS National Meeting, Anaheim, California, March 28 - April 1, 2004.

22. R.J. Kirkpatrick, A.G. Kalinichev, and J. Wang. Molecular dynamics modeling of mineral water interfaces. 227th ACS National Meeting, Anaheim, California, March 28 - April 1, 2004.
23. A.G. Kalinichev, J. Wang, and R.J. Kirkpatrick. Thermodynamics and structure of aqueous interfaces with layered inorganic solid phases: Molecular dynamics simulations. 3rd International Workshop "Global Phase Diagrams", Odessa, Ukraine, September 14-19, 2003.
24. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. Molecular structure of nano-confined water in brucite (001). 226th Annual Meeting of the American Chemical Society, New York City, NY, September 7-11, 2003.
25. R.J. Kirkpatrick, A.G. Kalinichev, and J. Wang. Molecular dynamics modeling of fluid-solid interactions in cement materials. European Congress and Exhibition on Advanced Materials and Processes, Lausanne, Switzerland, September 1-5 2003. (Keynote)
26. R.J. Kirkpatrick, A.G. Kalinichev, J. Wang, X. Hou, and J. Amonette. Molecular modeling of the vibrational spectra of interlayer and surface species of layered double hydroxides. Clay Minerals Society Workshop on "The Application of Vibrational Spectroscopy to Clay Minerals and Layered Double Hydroxides", Athens, GA, June 7-8, 2003. (Invited lecture).
27. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. Molecular modeling of water confined between hydrophilic surfaces of brucite. 40th Annual Meeting of Clay Minerals Society, Athens, GA, June 7-12, 2003.
28. A.G. Kalinichev, R.J. Kirkpatrick, and J. Wang. Molecular modeling of the interlayer H-bond networks in layered double hydroxides: structure and dynamics. 40<sup>th</sup> Annual Meeting of Clay Minerals Society, Athens, GA, June 7-12, 2003.
29. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. Molecular structure of water confined in brucite. 105th Annual Meeting of the American Ceramic Society, Nashville, TN, April 27-30, 2003.
30. A.G. Kalinichev, J. Wang, and R.J. Kirkpatrick. Molecular dynamics simulation of aqueous solutions confined in nano-pores and interlayers of inorganic materials. 225th Annual Meeting of the American Chemical Society, New Orleans, LA, March 23-27, 2003.
31. R.J. Kirkpatrick, A.G. Kalinichev, and J. Wang. Molecular modeling of aqueous fluids in nanospaces and at fluid-mineral interfaces. Surficial Geochemical Processes Symposia of Geosciences Research Program in DOE. Advanced Photon Source Conference Center, Argonne National Laboratory, March 7-8, 2003.
32. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. Structural ordering and dynamic deformation of hydrogen bond network in liquid water. EOS, Trans. Amer. Geophys. Union, 84, F1458, Fall AGU, 2002
33. A.G. Kalinichev, R.T. Cygan, J. Wang, and R.J. Kirkpatrick. Structure and dynamics of mineral/water interfaces: Molecular dynamics simulations of clays and clay-related phases. EOS, Trans. Amer. Geophys. Union, 84, F1396, Fall AGU, 2002.
34. J. Wang, A.G. Kalinichev, J.E. Amonette, and R.J. Kirkpatrick, 2002, Vibrational dynamics of Cl-hydroxalcalcite: A molecular dynamics modeling. AIChE Annual Meeting, Indianapolis, IN, November 3-8, 2002.
35. J. Wang, R.J. Kirkpatrick, A.G. Kalinichev, and J.E. Amonette. Interlayer structure and dynamics in Cl-Hydroxalcalcite: Far infrared spectroscopy and molecular dynamics modeling. 39th Annual Meeting of Clay Minerals Society, Boulder, Colorado, June 8-13, 2002.
36. J. Wang, A.G. Kalinichev, and R.J. Kirkpatrick. Hydration induced phase transitions of hydroxalcalcite: A molecular dynamics study. 39th Annual Meeting of Clay Minerals Society. Boulder, Colorado, USA. June 8-13, 2002.

37. A.G. Kalinichev, R.J. Kirkpatrick, and J. Wang. Hydration of carbonate-bearing species: Structure of aqueous  $\text{CO}_2$ ,  $\text{HCO}_3^-$ , and  $\text{CO}_3^{2-}$  from molecular dynamics computer simulations. EOS, Trans. Amer. Geophys. Union, 82, F1341 Fall AGU, 2001.
38. R.J. Kirkpatrick, A.G. Kalinichev, and J. Wang. Molecular dynamics modeling of water-solid interactions in cement systems. Materials Research Society 2001 Annual Meeting, Boston, MA, November 15-18, 2001. (Invited).
39. J. Wang, A.G. Kalinichev, R.J. Kirkpatrick and X. Hou. Molecular modeling of the interlayer structure and energetics of hydrotalcite hydration. 11th Annual V. M. Goldschmidt Conference, Hot Spring, Virginia, May 20-24, 2001.
40. R.J. Kirkpatrick, A.G. Kalinichev, X. Hou, J. Wang, H. Noma, and P. Yu. Structure and dynamics of layered double hydroxides: interlayer and surface species. 11th Annual V. M. Goldschmidt Conference, Hot Spring, Virginia, May 20-24, 2001. (Invited talk).
41. J. Wang, R.J. Kirkpatrick, A.G. Kalinichev, X. Hou, and J.E. Amonette. Far-infrared spectra of layered double hydroxides: experimental results and molecular dynamics simulation for hydrotalcite. 11th Annual V. M. Goldschmidt Conference. Hot Spring, Virginia, USA. May 20-24, 2001.
42. R.J. Kirkpatrick, A.G. Kalinichev, J. Wang, H. Noma, and X. Hou. Molecular modeling and NMR spectroscopy of carbonate species relevant to the geological sequestration of carbon dioxide. EOS, Trans. Amer. Geophys. Union, 81, F255-256. Fall AGU, 2000.
43. A.G. Kalinichev, J. Wang, and R.J. Kirkpatrick. Molecular simulations of fluids relevant to the geological sequestration of carbon dioxide. Geological Society of America Annual Meeting, Reno, Nevada, Nov. 12-16, 2000.
44. A.G. Kalinichev, J. Wang, R.J. Kirkpatrick, and R.T. Cygan. Molecular dynamics simulation of layered double hydroxides. FOMMS-2000 – First International Conference on Foundations of Molecular Modeling and Simulations, Keystone, CO, July 21-25, 2000.
45. A.G. Kalinichev, J. Wang, and R.J. Kirkpatrick. Ionic adsorption on the surface of hydroxides: A molecular dynamics study. 14th Symposium on Thermophysical Properties, Boulder, Colorado, June 25-30, 2000.
46. R.J. Kirkpatrick, A.G. Kalinichev, P. Yu, J. Wang, and X. Hou. Experimental NMR and molecular dynamics modeling of cement systems. 102nd Annual Meeting of the American Ceramic Society, St. Louis, Missouri, Apr.30 - May 3, 2000.
47. J. Wang, A.G. Kalinichev, R.J. Kirkpatrick, and X. Hou (2000) Molecular modeling of hydration in mixed metal layered hydroxides. 102nd Annual Meeting & Exposition of American Ceramic Society. St. Louis, Missouri, April 29 - May 3, 2000.
48. J. Wang, A.G. Kalinichev, R.J. Kirkpatrick, R.T. Cygan and X. Hou. Molecular modeling of the interlayer structure and dynamics in hydrotalcite. 9th Annual V. M. Goldschmidt Conference, Cambridge, Massachusetts, August 22-27, 1999.