

# Jianwei Wang

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## EDUCATION AND TRAINING

University of Michigan	Materials Science and Geochemistry	Postdoc	2007-2010
University of California	Geochemistry	Postdoc	2005-2006
University of Illinois	Geochemistry and Earth Materials	Ph.D.	1998-2004

## RESEARCH AND PROFESSIONAL EXPERIENCE

2013-present, Assistant Professor, Louisiana State University  
2011-2012, Assistant Research Scientist, University of Michigan  
2007-2010, Research Fellow, University of Michigan  
2005-2006, Postdoc Researcher, University of California at Davis  
1998-2004, Research Assistant, University of Illinois at Urbana-Champaign

## SYNERGISTIC ACTIVITIES

**Associate editor:** Frontiers – Earth and Planetary Materials (2014-)

**Referee of proposals for funding agencies:** Nuclear Energy University Program (NEUP), Office of Nuclear Energy, Department of Energy, Basic Energy Sciences, Office of Science, and Department of Energy.

**Conference committees and conveners:** Goldschmidt 2013, Florence, Italy. Theme 21 - Frontiers in Computational Geochemistry: Mineral Response to Extreme Conditions: Implications for the Nuclear Fuel Cycle. 2012: Judge for the best student presentation awards at Goldschmidt 2012, Montréal Canada.

**Referee for over 20 journals, including** Geochimica et Cosmochimica Acta, The Journal of Physical Chemistry, Physical Chemistry Chemical Physics, Journal of Molecular Modeling, Journal of American Ceramic Society.

**Guest scientist:** 2012-2017: Guangzhou Institute of Energy Conversion (GIEC), Chinese Academy of Sciences (CAS), member of International partners of Innovation Team.

## SCIENTIFIC HIGHLIGHTS AND MEDIA REPORTS

1. Science highlight from Journal of Physics: Condensed Matter on my published article. J. Physics: Condensed Matter, 23, 465503, 2011. “Site-split and band-shift under pressure”.  
<http://iopscience.iop.org/0953-8984/labtalk-article/47986>
2. A story: “A radioactive topic” by J. William Bell in the Access Magazine from TeraGrid and National Center for Supercomputing Applications (NCSA). 2009 Summer Edition. Print and online 8/25/2009.  
<http://web-test.ncsa.illinois.edu/News/Stories/Pyrochlores/>
3. Science Highlights from National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory highlight a paper in Physical Review Letters 100, 045503. Print and online 4/24/2009.  
[http://www.bnl.gov/ps/nsls/newsroom/publications/activityreport/2008\\_NSLs\\_Activity\\_Report.pdf](http://www.bnl.gov/ps/nsls/newsroom/publications/activityreport/2008_NSLs_Activity_Report.pdf)

4. Science Highlights from Consortium for Materials Properties Research in Earth Sciences (COMPRESS) highlight a paper in Physical Review Letters 100, 045503. Online 3/12/2008. [http://www.compres.us/index.php?option=com\\_content&task=blogcategory&id=45&Itemid=118](http://www.compres.us/index.php?option=com_content&task=blogcategory&id=45&Itemid=118)
5. A story: "Clearing the air". By J. William Bell in the Access Magazine. Print and online 10/03/2000. The National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign. <http://access.ncsa.illinois.edu/Stories/geochem/>

## PUBLICATIONS

### In press:

1. Tiankai Yao, Fengyuan Lu, Yachun Wang, Spencer Scott, Jianwei Wang, Rodney C. Ewing and Jie Lian (2014) Bulk Iodoapatite Ceramic Densified by Spark Plasma Sintering with Exceptional Thermal Stability. Journal of American Ceramic Society,

### Published:

2. J.W. Wang, R. C. Ewing, and U. Becker (2014) Average structure and local configuration of excess oxygen in  $\text{UO}_{2+x}$ . Scientific Reports, 04, 216. DOI:10.1038/srep04216.
3. F.X. Zhang, M. Lang, J.W. Wang, W.X. Li, K. Sun, V. Prakapenka, R.C. Ewing (2014) High-pressure  $\text{U}_3\text{O}_8$  with the fluorite-type structure. Journal of Solid State Chemistry, 213, 110.
4. J.W. Wang, R. C. Ewing, and U. Becker (2013) Electronic structure and stability of hyperstoichiometric  $\text{UO}_{2+x}$  under pressure. Physical Review B, 88, 024109.
5. J.W. Wang, M. Lang, R.C. Ewing, and U. Becker (2013) Multi-scale simulation of structural heterogeneity of swift-heavy ion tracks in complex oxides. Journal of Physics: Condensed Matter, 25, 135001. DOI: 10.1088/0953-8984/25/13/135001.
6. J.W. Wang and U. Becker (2013) Activation energetics of actinide diffusion in  $\text{UO}_2$  from first-principles calculations. Journal of Nuclear Materials, 433, 424-430. DOI: 10.1016/j.jnucmat.2012.10.011
7. F.N. Skomurski, J.W. Wang, R.C. Ewing, and U. Becker (2013) Charge distribution and oxygen diffusion in hyperstoichiometric uranium dioxide  $\text{UO}_{2+x}$  ( $x \leq 0.25$ ). Journal of Nuclear Materials, 434, 422-433. doi:10.1016/j.jnucmat.2011.09.003.
8. Fengyuan Lu, Jianwei Wang, Maik Lang, Marcel Toulemonde, Fereydoon Namavar, Christina Trautmann, Jiaming Zhang, Rodney C. Ewing and Jie Lian (2012) Amorphization of nanocrystalline monoclinic  $\text{ZrO}_2$  by swift heavy ion irradiation. Physical Chemistry Chemical Physics, 14, 12295–12300.
9. J.W. Wang and U. Becker (2012) Energetics and kinetics of carbonate orientational ordering in vaterite calcium carbonate. American Mineralogist, 97, 1427-1436.
10. H. Lu, J. W. Wang, C. Liu, C.I. Ratcliffe, and J.A. Ripmeester, (2012) Multiple  $\text{H}_2$  occupancy of the cages in hydrogen hydrate under mild condition. Journal of the American Chemical Society, 134, 9160-9162. DOI: 10.1021/ja303222u.
11. J.M. Zhang, J. Lian, F. Namavar, J.W. Wang, H. Haider, K. Garvin, and R.C. Ewing (2011) Nanosized Rutile ( $\text{TiO}_2$ ) Thin Film upon Ion Irradiation and Thermal Annealing. Journal of Physical Chemistry C, 115, 22755-22760, DOI: 10.1021/jp2056283
12. J.W. Wang, Z. Rak, F.X. Zhang, R.C. Ewing, and U. Becker (2011) Electronic structure and energetics of tetragonal  $\text{SrCuO}_2$  and its high-pressure superstructure phase. J. Physics: Condensed Matter, 23, 465503
13. J.W. Wang, F. Zhang, J. Lian, R.C. Ewing, and U. Becker (2011) Energetics of defect formation in  $\text{Gd}_2\text{Ti}_2\text{O}_7$  and  $\text{Gd}_2\text{Zr}_2\text{O}_7$  pyrochlore at high pressure. Acta Materialia 59,1607-1618.

14. J.W. Wang, H. Lu, J.A. Ripmeester, and U. Becker (2010) Molecular-Dynamics and First-Principles Calculations of Raman Spectra and Molecular and Electronic Structure of Hydrogen Clusters in Hydrogen Clathrate Hydrate. *Journal of Physical Chemistry C* 114, 21042-21050.
15. F.X. Zhang, J.W. Wang, M. Lang, J.M. Zhang, R.C. Ewing (2010) Pressure-induced structural transformations in lanthanide titanates:  $\text{La}_2\text{TiO}_5$  and  $\text{Nd}_2\text{TiO}_5$ . *Journal of Solid State Chemistry* 183, 2636-2643.
16. M. Lang, F.X. Zhang, J.M. Zhang, J.W. Wang, J. Lian, W.J. Weber, B. Schuster, C. Trautmann, R. Neumann, R.C. Ewing (2010) Review of  $\text{A}_2\text{B}_2\text{O}_7$  pyrochlore response to irradiation and pressure. *Nuclear Instruments and Methods in Physics Research B* 268, 2951–2959.
17. I. Sethmann, J.W. Wang, U. Becker, A. Putnis (2010) Strain-Induced Segmentation of Magnesian Calcite Thin Films Growing on a Calcite Substrate. *Crystal Growth & Design*, 10, 4319–4326. DOI: 10.1021/cg100202h.
18. J.M. Zhang, J. Lian, F.X. Zhang, J.W. Wang, A.F. Fuentes, and R.C. Ewing (2010) Intrinsic structural disorder and radiation response of nanocrystalline  $\text{Gd}_2(\text{Ti}_{0.65}\text{Zr}_{0.35})_2\text{O}_7$  pyrochlore. *Journal of Physical Chemistry C*, 114, 11810-11815.
19. F.X. Zhang, J.W. Wang, M. Lang, J.M. Zhang, R.C. Ewing (2009) High-pressure phase transitions of  $\text{ScPO}_4$  and  $\text{YPO}_4$ . *Physical Review B*, 80, 184114.
20. J. Wang, H. Lu, and J.A. Ripmeester (2009) Raman Spectroscopy and Cage Occupancy of Hydrogen Clathrate Hydrate from First-Principle Calculations. *Journal of the American Chemical Society*, 131, 14132-14133.
21. M. Lang, F. Zhang, J. Zhang, J. Wang, B. Schuster, C. Trautmann, R. Neumann, U. Becker, and R.C. Ewing (2009) Nanoscale manipulation of the properties of solids at high pressure with relativistic heavy ions. *Nature Materials*, 08, 793-797.
22. 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.
23. J. Wang and Udo Becker (2009) Structure and carbonate orientation of vaterite ( $\text{CaCO}_3$ ). *American Mineralogist*, 94, 380-386.
24. F. Zhang, M.K. Lang, J. Wang, U. Becker, and R.C. Ewing (2008) Structural phase transitions of cubic  $\text{Gd}_2\text{O}_3$  at high pressures. *Physical Review B*, 78, 064114.
25. 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  $\text{Gd}_2\text{Ti}_2\text{O}_7$  and  $\text{Gd}_2\text{Zr}_2\text{O}_7$  pyrochlores. *Physical Review Letters*, 100, 045503.
26. 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  $\text{SrCuO}_2$ . *Journal of the American Chemical Society*, 129, 13923-13926.
27. J. Wang, J.R. Rustad, and William H. Casey (2007) Water-exchange reactions on aluminous clays and minerals. *Inorganic Chemistry*, 46, 2962-2964.
28. 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.
29. 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.
30. 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.

31. Kirkpatrick R.J., Kalinichev A.G., Wang J., Hou X., and Amonette J.E. (2005) 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.
32. 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.
33. 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.
34. 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.
35. 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.
36. 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.
37. 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.
38. 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.

#### **PROCEEDINGS:**

39. J.D. Miller, V. Gupta, H. Du, X. Wang, X. Yin, and J. Wang (2011) "Surface Chemistry of Layered Silicate Minerals," in *Proceedings, Roe-Hoan Yoon International Symposium, 2011 SME Annual Meeting, Denver, Colorado, 27 February – 2 March 2011, SME, Littleton, Colorado*, pp. 289–298. Published, 03/2011.
40. J.W. Wang, R.C. Ewing, and U. Becker (2010). *Electronic Structure and the Energetics of Actinide Diffusion in UO<sub>2</sub>. Plutonium Futures—Science-2010*.
41. 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.

#### **BOOK AND BOOK CHAPTERS:**

42. R.C. Ewing, C. Huh, C. King and U. Becker, J. Wang, A.S. Donley, M.A. Wall, C.E. Krummrey, *Nanoscience & Nanotechnology Materials Survey: Applications to the Oil and Gas Industry*. September 2, 2009. Publisher: Advanced Energy Consortium (AEC), Houston, Texas 77041 and Bureau of Economic Geology, University of Texas, Austin, Texas 78758.

#### **INVITED TALKS:**

1. J.W. Wang. Computational Earth Materials for Environmental and Energy. *Molecular Simulations of Earth Materials for Environmental and Energy Applications*, HPC 3rd Annual HPC User Symposium. LSU Digital Media Center, Louisiana State University, June 4-5, 2014.
2. J.W. Wang. Multi-scale simulation of structural heterogeneity of swift-heavy ion tracks in complex oxides. *23rd International Conference on the Application of Accelerators in Research and Industry (CAARI 2014)*. San Antonio, Texas, USA. May 25-30, 2014

3. J.W. Wang. Computational Earth Materials for Environmental and Energy Applications. Department of Geology & Geophysics, Louisiana State University, Baton Rouge, Louisiana, March 18, 2013
4. J.W. Wang. Molecular modeling of earth materials and ceramics. Peking University, School of Engineering, Beijing, China, September 10, 2012.
5. J.W. Wang. Atomistic-scale understanding of water at mineral surfaces: Structure, dynamics, and energetics. Peking University, International Center for Quantum Materials, Beijing, China, September 7, 2012.
6. J.W. Wang. Molecular modeling of earth materials and ceramics. Guangzhou Institute of Energy Conversion(GIEC), Chinese Academy of Sciences(CAS), Guangzhou, China, September 3, 2012.
7. A.G. Kalinichev, J. Wang, and R.J. Kirkpatrick. Hydrogen bonding and molecular ordering of water at mineral-solution interfaces. (Keynote talk) Geochemical Society Goldschmidt Conference. Prague, Czech Republic. August 14-19, 2011.
8. J.W. Wang, H.L. Lu, and U. Becker. Structure and Vibrational Spectroscopy of Hydrogen Clusters in Hydrogen Clathrate Hydrate by Molecular Dynamics Simulation and First-Principles Calculation. (Invited talk) Geochemical Society Goldschmidt Conference 2010. Knoxville, Tennessee, June 13-18, 2010.
9. J.W. Wang. Structure, dynamics, and energetics at water and clay minerals interfaces by molecular modeling. Department of Metallurgical Engineering, the University of Utah. April 2010
10. J.W. Wang. Atomistic-scale understanding of water at mineral surfaces: Structure, dynamics, and energetics. Earth Science Division. Lawrence Berkeley National Laboratory, Berkeley, California. September, 2009.
11. J.W. Wang. Atomistic-scale understanding of water at mineral surfaces: Structure, dynamics, and energetics. Department of Geosciences, Stony Brook University, Stony Brook, New York. March 2007.
12. J.W. Wang. Understanding water interaction with ions, nanoparticles and mineral surfaces: structure, dynamics and energetics. University of Michigan, Ann Arbor, Michigan. May 2006.
13. J.W. Wang. Structure, dynamics and energetics of nano-confined water and water at mineral surfaces. Sandia National Laboratories, Albuquerque, New Mexico. June 2004.