

Blas P. Uberuaga

ADDRESS

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PROFESSIONAL PREPARATION

University of Idaho	Physics	B.A., 1994
University of Washington	Physics	Ph.D., 2000

APPOINTMENTS

2001-2004	Los Alamos National Laboratory, Postdoc
2004 – present	Los Alamos National Laboratory, Technical Staff Member

RESEARCH INTERESTS

Development of atomistic simulation methods. Application of those and other methods, including density functional theory, to problems in materials science, in particular radiation damage response and properties of point defects.

SELECTED PUBLICATIONS

- Uberuaga, B.P., Leskovar, M., Smith, A. P., Jonsson, H., and Olmstead, M., “Diffusion of Ge below the Si(100) Surface: Theory and Experiment,” *Physical Review Letters* **84**, 2441 (2000).
- Henkelman, G., Uberuaga, B. P., and Jonsson, H., “A climbing image nudged elastic band method for finding saddle points and minimum energy paths,” *Journal of Chemical Physics* **113**, 9901 (2000).
- Uberuaga, B. P., Voter, A. F., Sieber, K. K., and Sholl, D. S., “Mechanisms and Rates of Interstitial H₂ Diffusion in Crystalline C₆₀,” *Physical Review Letters* **91**, 105901 (2003).
- Uberuaga, B.P., Smith, R., Cleave, A.R., Montalenti, F., Henkelman, G., Grimes, R.W., Voter, A.F., and Sickafus, K.E., “Structure and mobility of defects formed from collision cascades in MgO,” *Physical Review Letters* **92**, 115505 (2004).
- Uberuaga, B.P., Anghel, M., and Voter, A.F., “Synchronization of trajectories in canonical molecular-dynamics simulations: Observation, explanation, and exploitation,” *Journal of Chemical Physics*, **120**, 6363 (2004).
- Uberuaga, B.P., Smith, R., Cleave, A.R., Henkelman, G., Grimes, R.W., Voter, A.F., and Sickafus, K.E., “Dynamical simulations of radiation damage and defect mobility in MgO,” *Physical Review B* **71**, 104102 (2005).

Smith, R., Bacorisen, D., Uberuaga, B. P., Sickafus, K. E., Ball, J. A., and Grimes, R. W., “Dynamical simulations of radiation damage in magnesium aluminate spinel, MgAl₂O₄,” *Journal of Physics: Condensed Matter* **17**, 875 (2005).

INVITED TALKS AT INTERNATIONAL MEETINGS

“Structure and mobility of defects formed in collision cascades in ceramics,” at the 2006 MMM meeting, Freiburg, Germany, September 2006 (upcoming)

“Applications of accelerated molecular dynamics in materials science,” at the 2006 ACS meeting, San Francisco, CA, September 2006 (upcoming)

“Structure and mobility of defects formed in collision cascades in ceramics,” at the 2006 TMS meeting, San Antonio, TX, March 12-16, 2006

“Spanning Time and Length Scales in Simulations of Radiation Damage,” at the 2005 MRS meeting, San Francisco, CA, March 28-April 1, 2005

“Molecular dynamics, molecular statics, and temperature accelerated dynamics study of radiation damage events and subsequent annealing in MgO,” at the 2004 COSIRES meeting, Helsinki, Finland, June, 2005

“Accelerated Dynamics Methods,” at the 2003 Electronic Structure meeting, Minneapolis, MN, May 2003

“Accelerated Dynamics Simulations of Carbon Nanostructures,” at the 2003 APS meeting, Austin, TX, March 2003

“Theoretical Investigations of Diffusion and Clustering in Semiconductors,” at the 2001 ICCN meeting, Hilton Head Island, SC, March, 2001

RECENT COLLABORATORS (4 years)

Jacques Amar (U. Toledo), Marian Anghel (LANL), Michael Baskes (LANL), Geoff Brown (LANL), Luciano Colombo (U. Cagliari), Tim German (LANL), Oyeon Kum (Clemson), Robin Grimes (Imperial College), John Hamilton (Sandia Livermore), Marilyn Hawley (LANL), Hannes Jonnson (U. Iceland), Joel Kress (LANL), X.-Y. Liu (RPI), Stuart Maloy (LANL), Francesco Montalenti (U. Milano), David Price (AWE), Lin Shao (LANL), David Sholl (Carnegie Mellon), Kurt Sickafus (LANL), Roger Smith (U. Loughborough), Jim Sprague (NRL), Srinivasan Srivilliputhur (LANL), Marius Stan (LANL), Steve Stuart (Clemson), Steve Valone (LANL), Arthur Voter (LANL), Wolfgang Windl (Ohio State).

GRADUATE AND POST-DOCTORAL ADVISORS

Hannes Jonsson, University of Washington (currently at the University of Iceland) (Ph.D.)

Arthur F. Voter, Los Alamos National Laboratory (postdoctoral)