

## ROUZBEH SHAHSAVARI (Biographical Sketch)

### PROFESSIONAL PREPARATION

Sharif University	Tehran	Civil Engineering	BS, 2002
McGill University	Montreal	Civil Engineering & Applied Mechanics	MS, 2004
MIT	Cambridge	Civil and Environment Engineering	PhD, 2011

### APPOINTMENTS

Assistant Professor, Rice University, Dept. of Materials Science and NanoEngineering.	2013-Present
Assistant Professor, Rice University, Dept. of Civil and Environmental Engineering	2011-Present
Research Assistant, Massachusetts Institute of Technology	2006-2011
Project Engineer, Excelsior Engineering Ltd., Calgary, AB.	2004-2006

### PUBLICATIONS

#### Publications in Relation to the Proposed Project

1. Abdolhosseini Qomi MJ, Krakowiak K, Bauchy M, Stewart K, **Shahsavari R.**, Jagannathan D, Brommera D, Baronnet A, Buehler M, Van Vliet K, Yip S, Ulm FJ, Pellenq R, (2014), Combinatorial Molecular Optimization of Calcium-Silicates, Nature Communications, 5:4960, DOI: [10.1038/ncomms5960](https://doi.org/10.1038/ncomms5960).
2. Pellenq R., Kushima A., **Shahsavari R.**, Van Vliet K., Buehler M., Yip S., Ulm F.-J., (2009), A realistic molecular model of calcium-silicate-hydrates, Proceedings of National Academy of Sciences of US, 09021180106, 1-6. DOI: [10.1073/pnas.0902180106](https://doi.org/10.1073/pnas.0902180106)
3. Muthuramalingam P., Sakhavand N., **Shahsavari R.**, (2013), H<sub>2</sub>, N<sub>2</sub> and CH<sub>4</sub> Gas Adsorptions in Zeolitic Imidazolate Framework-95, -100: Ab-initio Based Grand Canonical Monte-carlo Simulation, Journal of Physical Chemistry C, 117 (46), 24407-24416. DOI: [10.1021/jp408075y](https://doi.org/10.1021/jp408075y)
4. **Shahsavari R.**, Buehler M.J., Pellenq R., Ulm F.-J., (2009), First-principles study on elastic constants and interlayer interaction of complex hydrated oxides: case of tobermorite and jennite, Journal of American Ceramic Society, 92 (10) 2323-2330. DOI: [10.1111/j.1551-2916.2009.03199.x](https://doi.org/10.1111/j.1551-2916.2009.03199.x)
5. **Shahsavari R.**, Pellenq R., Ulm F.-J., (2011), Empirical force fields for complex calcio-silicate layered materials, Physical Chemistry Chemical Physics, 13, 1002-101. DOI: [10.1039/c0cp00516a](https://doi.org/10.1039/c0cp00516a).

#### Other Significant Products

1. Sakhavand N., **Shahsavari R.**, (2015), Universal Composition-Structure-Property Map for Natural and Biomimetic Platelet-matrix Composites and Stacked Heterostructures, Nature Communications, 6:6523, DOI: [10.1038/ncomms7523](https://doi.org/10.1038/ncomms7523).
2. Rafiee A., Narayanan T., Hashim D., Sakhavand N., **Shahsavari R.**, Vajtai R., Ajayan P.M., (2013), Hexagonal Boron Nitride and Graphite Oxide Reinforced Multifunctional Porous Composites, Advanced Functional Materials, 23, 5624-5630. DOI: [10.1002/adfm.201203866](https://doi.org/10.1002/adfm.201203866).
3. **Shahsavari R.**, Sakhavand N (2015), Junction Configuration-Induced Mechanisms Govern Elastic and Inelastic Deformations in Hybrid Carbon Nanomaterials, Carbon, 95, 699-709. DOI: [10.1016/j.carbon.2015.08.106](https://doi.org/10.1016/j.carbon.2015.08.106)
4. Jalilvand S., **Shahsavari R.**, (2015), Molecular Mechanistic Origin of Nanoscale Contact, Friction and Scratch in Complex Systems, ACS Applied Materials and Interfaces, 7 (5), 3362-3372. DOI: [10.1021/am506411h](https://doi.org/10.1021/am506411h)

5. **Shahsavari R.**, Chen L., (2015), Screw Dislocations in Complex, Low Symmetry Oxides: Core Structures, Energetics and Impacts on Crystal Growth, *ACS Applied Materials and Interfaces*, 7 (4), 2223-2234. DOI: 10.1021/am509808.

### SYNERGISTIC ACTIVITIES

1. **Development, Validation and Distribution of CSH-FF Force Field Potential:** I developed, validated and distributed the CSH-FF force field potential for Calcium-Silicates by simultaneously incorporating structural data and 21 elastic constants from *ab-initio* calculations. With high accuracy and simplicity, this force field potential has resulted in distribution to several research groups worldwide.
2. **Development of New Curricular Materials:** I developed a new graduate-level course, *Computational Nanoscience*, that is added to Rice's curriculum as a cross-disciplinary course in Materials Science and Civil Eng. This course teaches the basics of modern computational methods and their integration to sustainable design. Subjects include first principles, kinetic and classical Monte Carlo methods, Molecular Dynamics, Course Graining, Parallel Replica Exchange Dynamics, Metadynamics, and newly emerging theories for bridging time scales (e.g. autonomous basin climbing method).
3. **Peer Reviewer:** Langmuir, J. of Physical Chemistry C, Carbon, J. of Mechanics and Physics of Solids, J. of Applied Physics, Solid State Ionic, J. of American Ceramic Society, J. of Nanomechanics and Micromechanics, Computational Materials Science, Acta Bioamateriala, International Journal of Experimental and Computational Biomechanics, Materials and Structures, Materials Research Society Proceedings, J. of Engineering Mechanics, J. of Probabilistic Mechanics, Inorganic Chemistry Frontiers, International Journal of Experimental and Computational Biomechanics, Proposal reviewer and panelist at NSF, U.S. Army Corps of Engineers, and NASA.
4. **Professional Committee Service and Select Membership:** Materials Research Society (MRS), American Society of Mechanical Engineers (ASME), American Ceramic Society (ACER), Society of Engineering Sciences (SES), Engineering Mechanics Institute (EMI), International Association for Life-Cycle Engineering (IALCCE), Sigma Xi Society, etc.
5. **Student Mentoring Activities & Outreach to Under-represented Groups and Women:** Faculty fellow and Member, Rice-Houston Alliance for Graduate Education and the Professoriate (AGEP); Lecturer at 22nd Computer Modeling Workshop at National Institute of Standards and technology (NIST); Lecturer at "2012 Computational Modeling Tutorials" hosted by the American Ceramic Society; Advisor for female undergraduate and graduate students at Rice; Mentor and Judge in 2010 Entrepreneurship Contest at Harvard University; Outreach and mentoring underrepresented groups and women at Rice and Baylor College of Medicine at Houston.

### COLLABORATORS & OTHER AFFILIATIONS

**Collaborators:** Prof. Pulickel Ajayan, (Rice University), Prof. Adri van Duin (Pennsylvania State University), Dr. Akahior Kushima (MIT), Prof. Reza Shahbazian-Yasaar (Michigan State University), Prof. James Tour (Rice University), Prof. Krystyn VanVliet (MIT), Prof. Kenton Whitmire (Rice University), Prof. Emilie Ringe (Rice University), Prof. Sidney Yip (MIT), Dr. Prakash Muthuramalingam (University Paris East), Prof. Mathieu Bouchy (UCLA), Prof. Gurav Sant (UCLA), Prof. Abdolhosseini Qomi (UC, Irvine), Dr. Konrad Krakowiak (MIT). The total number of collaborators is 14.

**Graduate Advisors:** (3) Ph.D.: Prof. Markus Buehler (MIT) & Prof. Franz-Josef Ulm (MIT); M.S.: Prof. Martin Ostoja-Starzewski (University of Illinois at Urbana Champaign). The total number of graduate advisors is 3.

**Thesis Advisors and Postgraduate-Scholar Sponsor:** Dr. Sakineh E. Moghaddam (Post-doc at Rice), Dr. Sreepasad Srinivasam (Post-doc at Rice), Dr. Vahid Hejazi (Post-doc at Rice), Ross Warkentin (Ph.D student at Rice), Lei Tao (Ph.D student at Rice), Sung Hoon Hwang (Ph.D student at Rice), Joseph Carazzone (Ph.D student at Rice), Navid Sakhavand (Ph.D student at Rice; graduated in 2015), Shuo Zhao (MS student at Rice), Qi Zhang (MS student at Rice), Lu Chen (MS student at Rice; graduated in 2013). The total number of thesis advisors and postgraduate-scholar sponsors is 11.