

Biographical Sketch
Aravind R. Asthagiri
Assistant Professor
Department of Chemical Engineering
University of Florida

Professional Preparation:

The Ohio State University	B.S. Chemical Engineering Minor in Mathematics	May 1998
Carnegie Mellon University	Ph.D. in Chemical Engineering	May 2003
Geophysical Laboratory	Postdoctoral Fellow	July 2003-June 2005

Appointments:

Assistant Professor, Chemical Engineering, University of Florida July 2005 – present

Significant Publications:

1. A. Asthagiri and R.M. Hazen, "An *ab initio* Study of Adsorption of Alanine on the Chiral Calcite(21 $\bar{3}$ 1) Surface", *Molecular Simulation*, **33** 343-351 (2007).
2. A. Asthagiri and D.S. Sholl, "Pt Thin Films on Stepped SrTiO₃ Surfaces: SrTiO₃(620) and SrTiO₃(622)", *Journal of Molecular Catalysis A*, **216** 233-245 (2004).
3. T.D. Power, A. Asthagiri, and D.S. Sholl, "The Effect of Thermal Roughening on the Enantiospecificity of Naturally Chiral Pt Surfaces" *Langmuir*, **18** 3737-3748 (2002).
4. A. Asthagiri, P.J. Feibelman, and D.S. Sholl, "Thermal Fluctuations in the Structure of Naturally Chiral Pt Surfaces" *Topics in Catalysis*, **18** 193-200 (2002).
5. D.S. Sholl, A. Asthagiri, and T.D. Power, "Naturally Chiral Metal Surfaces as Enantiospecific Adsorbents" *Journal of Physical Chemistry B*, **105** 4771-4782 (2001).
6. S.R. Phillpot, S.B. Sinnott, and A. Asthagiri, "Atomic-Level Simulation of Ferroelectricity in Oxides: Current Status and Opportunities", *Annual Review of Materials Research*, **37** 239-270 (2007).
7. M. Ahart, A. Asthagiri, P. Dera, H-K. Mao, R. E. Cohen, and R. J. Hemley, "Single-domain electromechanical constants for Pb(Zn_{1/3}Nb_{2/3})O₃-4.5%PbTiO₃ from micro-Brillouin scattering", *Applied Physics Letters*, **88** 042908 (2006).
8. A. Asthagiri and D.S. Sholl, "Pt thin films on the polar LaAlO₃(100) surface: A First-principles study", *Physical Review B*, **73** 125432 (2006).
9. M. Ahart, A. Asthagiri, P. Dera, H-K. Mao, R. E. Cohen, and R. J. Hemley, "Single-domain electromechanical constants for Pb(Zn_{1/3}Nb_{2/3})O₃-4.5%PbTiO₃ from micro-Brillouin scattering", *Applied Physics Letters* **88** 042908 (2006).

10. A. Asthagiri, Z. Wu, N. Choudhury, R. E. Cohen, "Multiscale Modeling of Relaxor Ferroelectrics", *Ferroelectrics*, **333** 69-78 (2006).

Synergistic Activities:

1. Co-organized with Dr. Henry Teng a two-day symposium on Astrobiology/ Origin of Life at the Fall ACS National meeting in Philadelphia (2004).
2. Participated in NSF sponsored workshop on Computational Geoinformatics. Based on this workshop a summary of recommendations for future computational needs of the Earth Sciences community was compiled (2004).
3. Peer reviewed manuscripts for *Surface Science*, *Journal of Applied Physics*, *Journal of Molecular Catalysis A*, and *Catalysis Today*.
4. Co-chair of Session on Computational Modeling of Surfaces and Surface Phenomena at the AICHE National meeting in Cincinnati (2005, 2006). Co-coordinator of Area 1g (surface science) of the AICHE (2007-).
5. Member of recently formed Florida Society for Material Simulation. The goal of the society is to promote collaboration among researchers spanning all the universities in Florida.
6. Advisor for University of Florida AICHE Student Chapter. The UF Chapter won the Outstanding Student Award in 2006.

Collaborators:

Dr. Bob Downs	Dept. of Geosciences, Univ. of Arizona
Dr. Paul Salvador	Dept. of Material Science, Carnegie Mellon Univ.
Dr. Marcelo Sepiarsky	Instituto de Fisica Rosario
Dr. Russell Hemley	Carnegie Institution of Washington
Dr. Simon Phillpot	Dept. of Material Science & Engineering, Univ. of Florida
Dr. Susan Sinnott	Dept. of Material Science & Engineering, Univ. of Florida
Dr. Juan Nino	Dept. of Material Science & Engineering, Univ. of Florida
Dr. Jacob Jones	Dept. of Material Science & Engineering, Univ. of Florida
Dr. Jason Weaver	Dept. of Chemical Engineering, University of Florida

Postdoctoral Advisors

Dr. Robert Hazen	Carnegie Institution of Washington
Dr. Ron Cohen	Carnegie Institution of Washington

Thesis Advisor

Dr. David Sholl	Dept. of Chemical Eng., Carnegie Mellon Univ.
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Graduate Students

B. Brooks (Ph.D., current) and J. Hawkins (Ph.D., current)