

Biographical Sketch

Pushpa Raghani

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Professional Preparation

¹ JNCASR, Bangalore, India	Physics	Ph.D, 2006
Sardar Patel University, Anand, India	Physics	M. Phil., 1999
Gujarat University, Ahmedabad, India	Physics	M.Sc., 1998
C. U. Shah Science College, India	Physics	B.Sc., 1996

Appointments

2009 – Present: Assistant Professor of Physics, Boise State University, USA
2007 – 2009: Postdoctoral Researcher, Stanford University, USA
2006 – 2007: Postdoctoral Researcher, SISSA, Trieste, Italy
2005 – 2006: Research Assistant, SISSA, Trieste, Italy

Research Interests

Applications of *ab initio* Density Functional Theory, Density Functional Perturbation Theory and Nudged Elastic Band theory, in the following areas:

- Magnetic properties of transition metal atoms adsorbed on metal surfaces
- Chemical reactivity of clusters and surfaces
- Structural and dynamical properties of adsorbates on metal surfaces
- Structural, thermal and dynamical properties of small atomic clusters
- Reconstruction of homoepitaxial and heteroepitaxial metal surfaces

Publications

- “Thermodynamic stability of bi-layer of copper nitride on Cu(100) surface” Raghani Pushpa, Izaak Williamson, Barbara A. Jones, *J. Chem. Phys.* (2011, in Press)
- “Spin and exchange coupling for Ti embedded in a surface dipolar network” Raghani Pushpa, Jesus Cruz, Barbara A. Jones, *Phys. Rev. B*, **84** 075422 (2011)
- “Effective coordination number: A simple indicator of activation energies for NO dissociation on Rh(100) surfaces” Prasenjit Ghosh, Raghani Pushpa, Stefano de Gironcoli and Shobhana Narasimhan, *Phys. Rev. B*, **80** 233406 (2009)

¹ Jawaharlal Nehru Center for Advanced Scientific Research

- “Effective coordination as a predictor of adsorption energies: A model study of NO on Rh(100) and Rh/MgO(100) surfaces” Raghani Pushpa, Prasenjit Ghosh, Shobhana Narasimhan and Stefano de Gironcoli, *Phys. Rev. B*, **79** 165406 (2009)
- “Reconstruction of the second layer of Ag on Pt(111): Extended Frenkel-Kontorova model” Raghani Pushpa, Javier Rodriguez-Laguna, Silvia N. Santalla *Phys. Rev. B*, **79** 085409 (2009)
- “Interplay between bonding and magnetism in the binding of NO to Rh clusters”, Prasenjit Ghosh, Raghani Pushpa, Stefano de Gironcoli and Shobhana Narasimhan, *J. Chem. Phys.*, **128** 194708, (2008)
- “Bond Stiffening in small nanoclusters and its consequences for mechanical and thermal properties”, Raghani Pushpa, Umesh Waghmare and Shobhana Narasimhan, *Phys. Rev. B*, **77** 045427 (2008)
- “Subsurface oxygen stabilization by a third species: Carbonates on Ag(210)”, Letizia Savio, Andrea Gerbi, Luca Vattuone, Raghani Pushpa, Nicola Bonini, Stefano de Gironcoli and Mario Rocca, *J. Phys. Chem. C*, **111** 10923 (2007)
- $\text{Si}_x\text{C}_{1-x}\text{O}_2$ alloys: A possible route to stabilize carbon-based silica-like solids?”, Assa Aravindh et. al. *Solid State Comm.*, 144, 273-276, (2007)
- “Symmetry, Vibrational Instabilities and Origins of Structural Stability of Small Clusters of Al, Sn and As”, Raghani Pushpa, Shobhana Narasimhan and U. V. Waghmare, *J. Chem. Phys.*, **121** 5211 (2004)
- “The Reconstruction of Pt(111) and Domain Patterns on Close-packed Metal Surfaces”, Raghani Pushpa and Shobhana Narasimhan, *Phys. Rev. B*, **67** 205418 (2003)
- “Honeycombs, Triangles and Bright Stars: Pattern Formation on Metal Surfaces”, Shobhana Narasimhan and Pushpa Raghani, *Physics at Surfaces and Interfaces*, B.N. Dev (ed.), World Scientific, Singapore, pp 3-12 (2003)
- “Double Stripe Reconstruction of the Pt(111) Surface”, Raghani Pushpa and Shobhana Narasimhan, *Bull. Mater. Sci.* 26 1 (2003) (Conference Proceedings, Refereed)
- “Stars and Stripes: Nanoscale Misfit Dislocation Patterns on Surfaces”, Raghani Pushpa and Shobhana Narasimhan, *Pure Appl. Chem.* 74 1663 (2002) (Conference Proceedings, Refereed)

In Preparation

- Exchange coupling in dimers of Ti and Fe
- Vibrational Spectra of Si, Sn and Pb clusters

Synergistic Activities

- Invited Speaker: Summer conference and Workshop on: “Electronic Structure methods and their Applications”, International Quantum-ESPRESSO Meetings, JNCASR, Bangalore, India, July (2006)
- Invited Speaker: Material Science and Engineering seminar series, Boise State University, September (2010)

- Invited Speaker: Idaho Modeling, Simulation and Visualization Meeting, Boise State University, October (2010)
- Invited Speaker: Electronic structure of materials from first principles, Micron Technologies, Boise (2011)
- Research Supervisor of four undergraduate students at BSU
- Member of a “Mini-Development Grants Committee” at BSU
- Member of the “Physics Laboratory Committee” on improving the education in physics labs, BSU
- Graduate Faculty of BSU
- Reviewer for NSF grants

Teaching Activities

- Scientific Computing – phys325 at BSU (Fall 2009)
- Physics-I with calculus lab – phys211L at BSU (Spring 2010, Fall 2010)
- Modern Physics – phys311 at BSU (Fall 2010)
- Solid State Physics – phys415/515 at BSU (Spring 2011, Graduate Course)

Experience of working with graduate and undergraduate students

- Co-supervised two graduate (Ph.D.) students from Georgetown university on density functional theory
- Supervisor of four undergraduate students at Boise State University
- Co-supervisor of two graduate students at Boise State University

Talks and Posters

- Talk: Spin and exchange coupling in Ti atom and Ti dimer, Pittsberg, PA, USA (2009).
- Seminar: Spin and exchange coupling of Ti and Mn on Cu₂N/Cu(100) surface, Boise State University, USA (2009).
- Seminar: Adsorption of Ti and Mn on Cu₂N/Cu(100) surface, Stanford University (2008)
- Talk: Comparison between GGA+U and GGA-LSDA for Mn/CuN/Cu(100), New Orleans, Louisiana, USA (2008).
- Talk: Stabilization of subsurface oxygen by CO₃ on Ag(210), APS March meeting, Denver, Colorado, USA (2007).
- Talk: Effect of Rh coordination and surface stress on NO dissociation, APS March meeting, Denver, Colorado, USA (2007).
- Talk: Stabilization of Subsurface Oxygen by CO₃ on Ag(210), ELETTRA, Trieste, Italy (2006).

- Talk: Structural and Vibrational Consequences of Reduced Coordination, SISSA, Trieste, Italy.
- Thesis Colloquium: Structural and Vibrational Consequences of Reduced Coordination, JNCASR, (2004)
- Talk: Melting of Sn Clusters, JNCASR In-house Symposium.
- Talk: Anharmonic behaviour of Clusters through their Symmetry, Stability and Electronic Structure analysis, JNCASR.
- Talk: Reconstruction of the Pt(111) Surface, in the Winter college in Trieste, Italy.
- Seminar: One Dimensional Energy Dispersion of Single-Walled Carbon Nanotubes by Resonant Electron Scattering, JNCASR, Bangalore, India.
- Poster: Adsorption of Ti and Mn on CuN/Cu(100) Surface, Stanford University's Center for Probing the
- Poster: Adsorption of Ti and Mn on CuN/Cu(100) Surface, Stanford University's Center for Probing the Nanoscale (CPN), 4th Annual Workshop (2008)
- Poster: NanoItaly, Trieste, Italy (2006).
- Poster: Psik-2005 Conference (2005), Schwäbisch Gmünd, Germany.
- Poster: Workshop on Advanced Materials - II, Bangalore, India.
- Poster: ACCMS-1, Bangalore, India.

Awards

- Kawazoe-Aida prize for the best poster presentation in ACCMS-I, Bangalore, India.
- Postdoctoral fellowship, International School for Advanced Studies, SISSA, Italy
- Postdoctoral fellowship, Centre for Probing Nanoscale, Stanford University, USA