

## CURRICULUM VITAE

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### Academic History

Postdoc with Prof. Barbara Jones at Center for Probing the Nanoscale, Stanford University, Stanford, CA, USA (2007-Present).

Postdoc with Prof. Stefano de Gironcoli at SISSA, Trieste, Italy (2005-2007).

Ph.D. in Physics from 'Jawaharlal Nehru Centre for Advanced Scientific Research', in Theoretical Sciences Unit, with the thesis title "*Structural and Vibrational Consequences of Reduced Coordination*", supervised by Prof. Shobhana Narasimhan (JNCASR) (Awarded in 2006).

Master of Science in physics from *Gujarat University* Ahmedabad, India. (1998).

Bachelor of Science in physics from *C. U. Shah Science College* Ahmedabad, India (1996).

### RESEARCH INTERESTS

Applications of *ab initio* Density Functional Theory (DFT), Density Functional Perturbation Theory and Nudged elastic band theory, in the following areas:

- Exchange coupling in clusters of transition metal atoms
- 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 Metal Surfaces

### ONGOING PROJECTS

Exchange interactions in dimers of Fe and Ti deposited on CuN/Cu(100) surface (In collaboration with STM group of Dr. Andreas J. Heinrich at IBM Almaden Research Center)

Stark shift in quantum corrals (In collaboration with Prof. Hari Manoharan and Prof. Mark L. Brongersma at Physics department, Stanford University)

### PUBLICATIONS

"*Reconstruction of the second layer of Ag on Pt(111)*", Raghani Pushpa, Javier Rodriguez-Laguna, Silvia N. Santalla (arXiv:0810.2801; Accepted in PRB).

"*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)

"*Si<sub>x</sub>C<sub>1-x</sub>O<sub>2</sub> alloys: A possible route to stabilize carbon-based silica-like solids?*", Assa Aravindh et. al. *Solid State Comm.*, **144**, 273-276, (2007)

"*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)

“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). (Conference Proceedings, Refereed)

“Double Stripe Reconstruction of the Pt(111) Surface”, Raghani Pushpa and Shobhana Narasimhan, *Bull. Mater. Sci.* **26** 1 (2003) (Conference Proceedings, Refereed)

“Stars and Stipes: Nanoscale Misfit Dislocation Patterns on Surfaces”, Raghani Pushpa and Shobhana Narasimhan, *Pure Appl. Chem.* **74** 1663 (2002) (Conference Proceedings, Refereed)

## **UNDER REVIEW**

“Lowering Effective Coordination Promotes Adsorption of NO on Rh(100) and Rh/MgO(100) surfaces”, Raghani Pushpa, Prasenjit Ghosh, Shobhana Narasimhan and Stefano de Gironcoli (arXiv:0810.1910; Submitted to PRB)

## **IN PREPARATION**

Spin of Ti and Mn atoms on CuN/Cu(100)

Exchange coupling in dimers of Ti and Fe

Vibrational Spectra of Si, Sn and Pb clusters

Effects of strain and coordination on dissociation barrier of NO on Rh(100)

## **PROGRAMS USED**

QUANTUM-ESPRESSO (DFT program based on pseudopotentials and plane waves)

WIEN2K (DFT program based on all electron methods)

XCrySDen (Crystalline and molecular structure visualisation program)

## **PROGRAMMING LANGUAGES**

Fortran 90, 95, C++

## **TEACHING EXPERIENCE**

I have taught in the “SUMMER SCHOOL ON ELECTRONIC STRUCTURE METHODS AND APPLICATIONS, AND WORKSHOP ON COMPUTATIONAL MATERIALS THEORY”, held at JNCASR, Bangalore, India, July 2006.

## **TALKS AND POSTERS**

Poster: Adsorption of Ti and Mn on CuN/Cu(100) Surface, Stanford University’s Center for Probing the Nanoscale (CPN), 4th Annual Workshop (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 CO<sub>3</sub> 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).

Poster: NanoItaly, Trieste, Italy (2006).

Talk: Stabilization of Subsurface Oxygen by CO<sub>3</sub> on Ag(210), ELETTRA, Trieste, Italy (2006).

Poster: Psik-2005 Conference (2005), Schwabisch Gmünd, Germany.

Talk: Structural and Vibrational Consequences of Reduced Coordination, SISSA, Trieste, Italy.

Thesis Colloquium: Structural and Vibrational Consequences of Reduced Coordination, JNCASR.

Talk: Melting of Sn Clusters, JNCASR In-house Symposium.

Talk: Anharmonic behaviour of Clusters through their Symmetry, Stability and Electronic Structure analysis, JNCASR.

Poster: Workshop on Advanced Materials - II, Bangalore, India.

Talk: Reconstruction of the Pt(111) Surface, in the Winter college in Trieste, Italy.

Poster: ACCMS-1, Bangalore, India.

Seminar: One Dimensional Energy Dispersion of Single-Walled Carbon Nanotubes by Resonant Electron Scattering, JNCASR, Bangalore, India.

**AWARDS** Kawazoe-Aida prize for the best poster presentation in ACCMS-I, Bangalore, India.