

Curriculum Vitae: Madhura Marathe

Marie-Curie (COFUND) postdoctoral fellow,
ICMAB-CSIC, Campus de la UAB,
08193 Bellaterra,
Barcelona, Spain.

e-mail: mmarathe@icmab.es
Phone: +34 935 801 853 (Ext. 288)
Fax: +34 935 805 729

Date of Birth: April 1984
Sex: Female
Nationality: Indian.

Educational Qualifications

- 2006-2013: Ph.D. research,
J. N. Centre for Advanced Scientific Research, Bangalore, India.
Thesis: "Structural, magnetic and electronic properties of surface alloys
and interfaces: A first-principles study"
Advisor: Prof. Shobhana Narasimhan.
- 2004-2006: Master of Science (M.Sc. in Physics)
Department of Physics, University of Pune, Pune, India.
- 2001-2004: Bachelor of Science (B.Sc. in Physics)
Fergusson college, University of Pune, Pune, India.

Research Experience

- Jul. 2017: Marie-Curie (COFUND) postdoctoral fellow,
Institut de Ciència de Materials de Barcelona (ICMAB-CSIC),
Mentor: Dr. Massimiliano Stengel.
- Sept. 2013 - Mar. 2017: Post-doctoral Fellow, Materials Theory, ETH Zürich.
Mentors: Prof. Nicola Spaldin and Prof. Dr. Claude Ederer.

Research Interests

- Application of **density functional theory** to study structural, magnetic and electronic properties of metallic surface alloys and interfaces as well as properties of ferroelectric materials.
- Use of **molecular dynamics simulations for a coarse-grain effective Hamiltonian** to calculate finite temperature properties, e.g., calculation of temperature-strain phase diagram for epitaxially strained BaTiO₃.
- Study of **the electrocaloric effect** focussing on the comparison between the direct and indirect methods, and understanding the anisotropy of the effect as well as tuning the temperature change by applying strain.
- Application of cluster expansion technique and Frenkel-Kontorova model to study large systems inaccessible within DFT such as alloys with a small concentration of substitutional atoms and surface reconstructions.

Technical Skills

- Programming in FORTRAN and matlab.
- Density functional theory calculations using Quantum-ESPRESSO, abinit and VASP codes.
- Molecular dynamics simulations for a coarse-grain model using “feram” code.
- Shell scripting.
- Good knowledge of Xcrysden, gnuplot and xmgrace.

Teaching Experience

- Mentoring two master student projects (8 week duration): Damian Renggli and Jonathan Spring.
- Teaching Assistant for “solid state physics and chemistry of materials” in 2014 and 2016 at ETH-Zürich.
- Tutor for MASTANI (MAterials Simulations Theory And numerIcs) summer school in June-July 2014 at Pune, India.
- Teaching assistant for JT201 (Introductory Solid State Physics) course in 2008 and 2009 at JNCASR.
- Designed exercise 2 of the tutorial (calculation of band structure of Si and post-processing) for Summer school on Materials modeling from first principles: theory and practice, ICMR, University of California at Santa Barbara, July 2009.
- Tutor for JNCASR/SISSA/IBM School on First-Principles Simulations Nov. - Dec. 2009 (Designed and conducted a tutorial on simple SCF ground state calculations, band structures, DOS using Quantum-ESPRESSO).

Distinctions and Awards

- Finalist in Nottingham Prize Competition held at PEC2010, University of Wisconsin, Milwaukee, USA, June 2010.
- Best poster prize at 2nd International Conference on Physics at Surfaces and Interfaces, Puri - India, February 2009.

Other Activities

- Helped to prepare and present renewal of funding proposal for DFG priority program on Ferroic cooling (SPP 1599) as well as presented part of our work to other research groups during internal meetings which enable possible collaborations within the focus program.
- Reviewed articles as a referee.

List of Publications

1. “The impact of hysteresis on the electrocaloric effect at first-order phase transitions”, Madhura Marathe, C. Ederer and A. Grünebohm, *Phys. Status Solidi B* **255**, 1700308 (2018).
2. “The electrocaloric effect in BaTiO₃ at all three ferroelectric transitions: anisotropy and inverse caloric effects”, Madhura Marathe, D. Renggli, M. Sanlialp, M. O. Karabasov, V. V. Shvartsman, D. C. Lupascu, A. Grünebohm and C. Ederer, *Phys. Rev. B* **96**, 014102 (2017).
3. “Tuning the caloric response of BaTiO₃ by tensile epitaxial strain”, A. Grünebohm, Madhura Marathe, C. Ederer, *Europhys. Lett.* **115**, 47002 (2016).
4. “First-principles-based calculation of the electrocaloric effect in BaTiO₃: A comparison of direct and indirect methods”, Madhura Marathe, A. Grünebohm, T. Nishimatsu, P. Entel and C. Ederer, *Phys. Rev. B* **93**, 054110 (2016).
5. “*Ab initio* phase diagram of BaTiO₃ under epitaxial strain revisited”, A. Grünebohm, Madhura Marathe and C. Ederer, *Appl. Phys. Lett.* **107**, 102901 (2015).
6. “Electrocaloric effect in BaTiO₃: A first-principles-based study on the effect of misfit strain”, Madhura Marathe and C. Ederer, *Appl. Phys. Lett.* **104**, 212902 (2014).
7. “Ab Initio and Cluster Expansion Study of Surface Alloys of Fe and Au on Ru(0001) and Mo(110): Importance of Magnetism”, Madhura Marathe, A. Díaz-Ortiz and S. Narasimhan, *Phys. Rev. B* **88**, 245442 (2013).
8. “Spin-polarized Surface States on Fe-deposited Au(111) surface: a theoretical study”, Madhura Marathe, J. Lagoute, V. Repain, S. Rousset and S. Narasimhan, *Surf. Sci.* **606**, 950 (2012).
9. “Prediction of Reconstruction in Heteroepitaxial Systems using the Frenkel-Kontorova Model”, S. Mehendale, Madhura Marathe, Y. Girard, V. Repain, C. Chacon, J. Lagoute, S. Rousset and S. Narasimhan, *Phys. Rev. B* **84**, 195458 (2011).
10. “Electronic properties of Fe clusters on a Au(111) surface”, A. Delga, J. Lagoute, V. Repain, C. Chacon, Y. Girard, Madhura Marathe, S. Narasimhan and S. Rousset, *Phys. Rev. B* **84**, 035416 (2011).
11. “Ordered Surface Alloy of Bulk-immiscible Components Stabilized by Magnetism”, S. Mehendale, Y. Girard, V. Repain, C. Chacon, J. Lagoute, S. Rousset, Madhura Marathe and S. Narasimhan, *Phys. Rev. Lett.* **105**, 056101 (2010). (Selected as Editor’s Suggestion)
12. “Mixing and Magnetic Properties of Surface Alloys: The Role of the Substrate”, Madhura Marathe, M. Imam and S. Narasimhan, *Appl. Surf. Sci.* **256**, 449 (2009).
13. “Ni_xPt_{1-x}/Rh(111): A Stable Surface Alloy with Enhanced Magnetic Moments”, M. Imam, Madhura Marathe and S. Narasimhan, *Solid State Comm.* **149**, 559 (2009).
14. “Elastic and Chemical Contributions to the Stability of Magnetic Surface alloys on Ru(0001)”, Madhura Marathe, M. Imam and S. Narasimhan, *Phys. Rev. B* **79**, 085413 (2009).
15. “Competition between Elastic and Chemical Effects in the Intermixing of Co and Ag on Rh(111)”, M. Imam, Madhura Marathe and S. Narasimhan, *J. Chem. Sci.* **120**, 621 (2008).
16. “Si_xC_{1-x}O₂ Alloys: A possible route to stabilize carbon-based silica-like solids?”, A. Aravindh, *et al.*, *Solid State Comm.* **144**, 273 (2007).

Presentations and Talks

1. ISAF/ECAPD/PFM Conference, Darmstadt, Germany, August, 2016 (oral).
2. DPG spring meeting, Regensburg, Germany, March 2016 (oral).
3. Psi-K conference, San Sebastian, Spain, September 2015 (poster).
4. Joint ISAF-ISIF-PFM conference, Singapore, May 2015 (oral).
5. DPG spring meeting, Dresden, Germany, April 2014 (oral).
6. Workshop on the Fundamental Physics of Ferroelectrics and Related Materials, Washington D.C., USA, January 2014 (oral).
7. International Conference on Nanoscience + Technology (ICN+T), Paris, France, July 2012 (oral).
8. 15th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy, January 2011 (poster).
9. Physical Electronics Conference on the Physics and Chemistry of Surfaces and Interfaces, University of Wisconsin, Milwaukee, USA, June 2010 (oral).
10. JNCASR conference on Chemistry of Materials, Alleppey - India, October 2009 (oral and poster).
11. 2nd International Conference on Physics at Surfaces and Interfaces, Puri - India, February 2009 (poster).

Schools attended

- Essentials for Scientific Computing, Centre for Computational Materials Science, JNCASR, May 2012.
- Bangalore Summer School on Electronic Structure Methods and their Applications in conjunction with Conference on Computational Materials Theory, JNCASR, July 2006.