Priya Mahadevan

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Professor Priya Mahadevan is a Condensed Matter theorist working on understanding how materials behave using both ab-initio as well as model Hamiltonian calculations.

Supervision of Research / Students

Ph.D. Students

1. Shishir Kumar Pandey; Unusual magnetic ground states in transition metal oxides; Ongoing
2. Sagar Sarkar; Role of structure in determing the properties of transition metal oxides; Ongoing
3. Poonam Kumari; Spin orbit effects in the properties of low-dimensional semiconductors; Ongoing
4. Joydeep Chatterjee; Electronic structure of low dimensional semiconductors; Ongoing
5. Sumanti Patra; Optical properties of layered transition metal dichalcogenides; Ongoing

Publications in Journals

1. Soumyadipta Pal, Sagar Sarkar, Shishir Kumar Pandey, Chhayabrota Maji and **Priya Mahadevan;** *Driving force for martensitic transformation in* $Ni_2Mn_{1+x}Sn_{1-x}$; Phys. Rev B; 2016; **94;** 115143.
2. M. Mittal, A. Jana, S. Sarkar, **Priya Mahadevan** and Sameer Sapra; *Size of the organic cation tunes the band gap of colloidal organolead bromide perovskite nanocrystals;* J. Phys. Chem. Lett.; 2016; **7;** 3270.
3. S. Middey, J. Chakhalian, **Priya Mahadevan,** JW. Freeland, AJ Millis and D.D. Sarma; *Physics of ultrathin films and heterostructures of rare-earth nickelates;* Ann Rev of Mat. Res.; 2016; **46;** 305.
4. S. Middey, P, Aich, C. Meneghini, K. Mukherjee, E.V. Sampathkumaran, V. Siriguri, **Priya Mahadevan** and Sugata Ray; *Metal-insulator transition in* $Ba_3Fe_{1-x}Ru_{2+x}O_9$*: Interplay between site disorder, chemical percolation, and electronic structure;* Phys. Rev. B; 2016; **94;** 184424.

Lectures Delivered

1. 2nd Lakshmi Raman memorial lecture, IIT Madras, April 2016.
2. ICAMMP VI, IIT Kharagpur, November 2016.
3. AESET 2016, Puri, December 2016.
4. PCOTE 2017, Kolkata, January 2017.
5. ICAFM 2017, Chennai, January 2017.
6. WCMP 2017, IIT Kharagpur, February 2017.
7. JNU March meeting, JNU Delhi, March 2017.

Membership of Committees

External Committee

IUPAP National Committee; IUPAP C20 Commission on Computational Physics; various SERB review committees

Internal Committee

Various thesis committees, SCOLP, CWEP

Fellow / Member of Professional Body

1. Fellow of Indian Academy of Science

Sponsored Projects

1. Functional transition metal oxides, DAE-BRNS, 2014-2017

Conference / Symposia / Workshops / Seminars etc. organized

1. MRSI Young scientist meet, September 2016, SN Bose centre, Co-convener

Collaborations including publications (Sl. No. of paper/s listed in 'Publications in Journals' jointly published with collaborators)

National

Sl. No. 1, 2, 4

International

Sl. No. 3

Significant research output / development during last one year

General research areas and problems worked on

Understanding the martensitic transition in shape memory alloys; Role of the cation at the A site of a perovskite of the form ABX_3 in determining the structure and properties of the perovsite

Interesting results obtained

The ideas of how the ionic size of the atom at the A site of a perovskite of the form ABX_3 are well understood. However, a recent class of materials that have been of interest for photovoltaic applications have a molecule at the A site. The question is how does the size of the molecule determine the structure and consequently the electronic properties of these materials. A part of this question has been addressed in JPCL 7, 3270 (2016).As in the inorganic perovskites the atom/molecule at the A site of the perovskite lattice ABX3 plays an important role in determining the size of the unit cell as well as the structural distortions. What we go on to show is that these two have differing effects on the band gap of the system. The literature so far has not distinguished the various contributions such as volume, structural distortions etc and this has led to ambiguity in the role of the cation at the A site which we clarify for the first time in these systems.

The shape memory alloys of the form Ni-Mn-Sn exhibit a transition from the high symmetric cubic phase only for non-stoichiometric compositions. Our first principle electronic structure calculations are able to capture the transition that takes place for only certain compositions. We are therefore able to discuss what are the microscopic considerations that drive the transition. This has appeared in Phys. Rev. B 94, 115143 (2016).

Proposed research activities for the coming year

We had presented a heuristic model in 2004 to understand the magnetism in dilute magnetic semiconductors based on an analysis of various features and trends that we had found in the electronic structure and magnetic properties calculated within an ab-initio framework. We are now developing a microscopic model within a model Hamiltonian framework to extend the purview of these results and examine various limits.

Another unusual feature that we are trying to understand are the glassy dynamics of hybrid perovskites seen in the low temperature orthorhombic phase where one expects the molecular dipoles to be frozen in and no other form of crystallographic disorder is believed to be present.