

## Dr. Mukul Kabir

### Senior Postdoctoral Research Associate

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### Positions :

- Nov, 2009 - : *Senior Postdoctoral Research Associate*  
Department of Materials Science and Engineering  
Massachusetts Institute of Technology, USA
- Dec, 2006 - Nov, 2009 : *Postdoctoral Research Associate*  
Advisor: Prof. Krystyn J. Van Vliet  
Department of Materials Science and Engineering  
Massachusetts Institute of Technology, USA
- March, 2006 - May, 2006 : *Visiting Researcher*  
Department of Physics, Uppsala University, Sweden
- 2003 - 2006 : *Senior Research Fellow*  
S. N. Bose National Center for Basic Sciences, India
- 2001 - 2003 : *Junior Research Fellow*  
S. N. Bose National Center for Basic Sciences, India

### Academic :

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| Ph.D. (Physics)                              | 2006        | S. N. Bose National Centre for Basic Sciences, Kolkata, India |
| Graduate Aptitude Test in Engineering (GATE) | 2001        | Department of Education, MHRD, India                          |
| M. Sc. in Physics                            | 1998 - 2000 | University of Calcutta, Kolkata, India                        |
| B. Sc. in Physics                            | 1995 - 1998 | University of Calcutta, Kolkata, India                        |

### Research :

- Broad : Multiscale materials modeling  
(i) Density functional theory based electronic structure calculation, (ii) Reaction pathways using Nudged elastic band method, (iii) Molecular dynamics, (iv) Lattice thermodynamics, (v) kinetic Monte Carlo.
- Specific
- Modeling of (point/extended) defect kinetics in Fe-C alloy
  - Reversible photoinduced magnetism in prussian blue analogs
  - Adsorption pathways of O<sub>2</sub>, CO<sub>2</sub>, CO, and NO on Fe-Porphyrin.
  - Magnetic properties of pure and doped transition metal clusters
  - Magnetism in spintronic (Mn/Co/Cr)-ZnO material.
  - Dissociative H<sub>2</sub> adsorption in V<sub>n</sub>@Co<sub>m</sub> cluster.
  - Electronic structure of biological molecules

Methods	<ul style="list-style-type: none"> <li>• Density Functional Theory (LDA, GGA, GGA+U)</li> <li>• Nudged Elastic Band (NEB)</li> <li>• kinetic Monte Carlo (kMC)</li> </ul>
Code	I have extensively used the Vienna <i>ab initio</i> Pseudopotential Package (VASP).
Code developed	Tight-Binding molecular dynamics code (during my Ph.D.), Nudged Elastic Band (NEB) and kinetic Monte Carlo (kMC) codes at MIT.
Programming skill	Fortran 77, Fortran 90, Shell Script

**Ph. D. Thesis :**

Title	Electronic and Magnetic Properties of Metal Clusters. (2006) S. N. Bose National Center for Basic Sciences, Kolkata, India
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**Preprints:**

1. **Mukul Kabir**, T. T. Lau, S. Yip, and Krystyn J. Van Vliet  
*Predicting Dislocation Mobility from Explicit Atomistic Details: A Kinetic Monte Carlo Study*  
Communicated for publications (2010)
2. **Mukul Kabir**, T. T. Lau, Xi Lin, S. Yip, and Krystyn J. Van Vliet  
*Effects of vacancy-solute point defect clusters on diffusivity in metastable Fe-C alloys*  
Communicated for publication (2010).
3. **Mukul Kabir**, and Krystyn J. Van Vliet  
*Origin of photoinduced magnetization in Prussian blue analog*  
In preparation (2010)

**Publications in refereed journals :**

1. S. Datta, **Mukul Kabir**, Abhijit Mookerjee, and Tanusri Saha-Dasgupta  
*Structure, reactivity and electronic properties of V-doped Co clusters*  
**Physical Review B 80, 085418 (2009)**
2. Diana Iusan, **Mukul Kabir**, Olle Eriksson, and Biplab Sanyal  
*A microscopic picture of Co clustering in ZnO*  
**Physical Review B 79, 125202 (2009)**
3. Soumendu Datta, **Mukul Kabir**, Tanusri Saha-Dasgupta, and D. D. Sarma  
*Study of Structural Stability and Electronic Structure of Nonstoichiometric CdS Nano Clusters from First Principles*  
**Journal of Nanoscience and Nanotechnology 9, 5489 (2009)**
4. S. Ganguly, **Mukul Kabir**,\* S. Datta, B. Sanyal, and A. Mookerjee  
Magnetism in small bimetallic Mn-Co clusters  
**Physical Review B 78, 014402 (2008)**  
This paper was featured in the **Virtual Journal of Nanoscale Science & Technology, Vol-18, Issue-2 (2008)**. \*Corresponding author

5. S. Datta, **Mukul Kabir**, T. Saha-Dasgupta, and D. D. Sarma  
*First principle study of structural stability and electronic structure of CdS nanoclusters*  
**J. Physical Chemistry C** **112**, 8206 (2008)
6. S. Samanta, **Mukul Kabir**, B. Sanyal and D. Bhattacharya  
*Twist dependent staking energy of base-pair step: A density functional theory approach*  
**Int. J. Quantum Chemistry** **108**, 1173 (2008)
7. **Mukul Kabir**, D. G. Kanhere and Abhijit Mookerjee  
*Emergence of noncollinear magnetic ordering in small magnetic clusters:  $Mn_n$  and  $As@Mn_n$*   
**Physical Review B** **75**, 214433 (2007)
8. S. Datta, **Mukul Kabir**,\* S. Ganguly, B. Sanyal, T. Saha-Dasgupta, and A. Mookerjee  
*Structure, bonding, and magnetism of cobalt clusters from first-principles calculations*  
**Physical Review B** **76**, 014429 (2007). \*Corresponding author
9. **Mukul Kabir**, Abhijit Mookerjee and D. G. Kanhere  
*Structure, electronic properties and magnetic transition in manganese clusters*  
**Physical Review B** **73**, 224439 (2006)  
This paper was featured in the **Virtual Journal of Nanoscale Science & Technology**,  
**Vol-14, Issue-2 (2006)**.
10. **Mukul Kabir**, D. G. Kanhere and Abhijit Mookerjee  
*Large magnetic moments and anomalous exchange coupling in As-doped Mn clusters*  
**Physical Review B** **73**, 75210 (2006)
11. **Mukul Kabir**, Abhijit Mookerjee and A. K. Bhattacharya  
*Structure and stability of Cu clusters : A tight-binding molecular dynamics study.*  
**Physical Review A** **69**, 043203 (2004)
12. **Mukul Kabir**, Abhijit Mookerjee and A. K. Bhattacharya  
*Copper clusters : Electronic effect dominates over geometrical effect*  
**European Physical Journal D** **31**, 477 (2004)
13. **Mukul Kabir**, Abhijit Mookerjee, R. P. Datta, Amitava Banerjea and A. K. Bhattacharya  
*Study of small metallic nanoparticles : An ab-initio full-potential muffin-tin orbitals based molecular dynamics study of small Cu clusters.*  
**Int. J. of Mod. Phys. B** **17**, 2061, (2003)

### Publications in Proceedings:

1. **Mukul Kabir**, Abhijit Mookerjee, and D. G. Kanhere  
Magnetism in pure and doped manganese clusters.  
*Lecture series on computer and computational sciences*, Vol-4 pp 1018-1021 (Brill Academic Publishers, The Netherlands, 2005)
2. **Mukul Kabir**, and Abhijit Mookerjee  
Tight-Binding Molecular Dynamics Study of Copper Clusters  
*Nano-Scale Materials: From Science to Technology* Eds., S.N.Sahu, R.K. Choudhury and P. Jena (Nova, New York, 2006)

**Chapters in Books:**

1. **Mukul Kabir**, Abhijit Mookerjee, and D. G. Kanhere  
Magnetism in pure and doped manganese clusters  
Astrophysics and Condensed Matter: Horizons in World Physics (Vol. 262, Nova, New York, 2008).

**Invited lectures :**

1. *Magnetic ordering in small magnetic clusters*  
Uppsala University, Sweden, 20 April, 2006
2. *Emergence of noncollinear magnetic ordering in pure and As-doped manganese clusters*  
International Conference of Computational Methods in Sciences and Engineering.  
Korinthos, Greece, 21-26 October 2005
3. *Electronic and magnetic properties of pure and doped manganese clusters*  
University of Saarland, Germany, 19 October, 2005

**Significant presentations in conferences/workshops :****Lectures**

1. *Atomistic modeling of dislocation mobility* at the American Physical Society Meeting, Portland, March 15-19, 2010.
2. *Predicting Dislocation Mobility From Explicit Atomistic Details* at the TMS Annual Meeting, Seattle, February 14-18, 2010.
3. *Novel Mechanism of Reversible Photoinduced Magnetism in Prussian Blue Analogs* at the Materials Research Society meeting, Boston, November 30 - December 3, 2009.
4. *Predicting Dislocation Mobility From Explicit Atomistic Details: A Kinetic Monte Carlo Study* at the Materials Research Society meeting, Boston, November 30 - December 3, 2009.
5. *Point defect diffusion and dislocation climb in ferritic steel* at The Fourth International Conference on Multiscale Materials Modeling (MMM-2008), Tallahassee, Florida, 27-31 October, 2008
6. SERC School on Condensed Matter Physics, Saha Institute of Nuclear Physics, Kolkata, India 02 - 31 January, 2006

**Posters**

1. *Novel mechanism of reversible spin transition in Prussian Blue analogs* at the the American Physical Society Meeting, Portland, March 15-19, 2010.
2. Indo-US Conference on Novel and Complex Materials, S. N. Bose National Center for Basic Sciences, 26 - 29 October, 2006
3. Third Indo-Israel meeting, Hotel Toshali Sands, Puri, India, 17 - 21 April, 2005
4. Indo-US Workshop on Nano-scale Materials: From Science to Technology, Hotel Mayfair, Puri, India, 5-8 April, 2004

5. Workshop and conference on physics, of novel materials: Electronic and magnetic properties, S. N. Bose National Center for Basic Sciences, 05 - 14 January, 2004
6. International Conference on Nano Science and Technology, Hyatt Regency, Kolkata, 17-20 December 2003

### **Other Responsibilities**

Referee	Physica B
Full Member	Sigma Xi, The Scientific Research Society, 2009
Member	American Physical Society
Member	Materials Research Society

**Total Citation:** 110+