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EDUCATIONAL BACKGROUND

- Ph. D., IACS, Kolkata (1999)
- M. Sc.(Physics), University of Calcutta (1992)

RESEARCH INTERESTS

- Complex electronic and magnetic phenomena in strongly correlated TM oxides
- Understanding of electron-transfer related processes in biological macromolecules
- Electronic structure and transport in 1D/2D organic conductors
- Prediction and engineering of magnetism in 2 dimensional systems like graphene
- Numerical calculation of optical properties, namely optical conductivity, reflectivity, magneto-optical Kerr rotation spectrum in materials.

AWARDS/FELLOWSHIPS

- Associateship at S. N. Bose National Centre for Basic Sciences, Aug 2012- Aug 2015
- DST- WOS(A) Fellowship, 2006
- CSIR JRF-LS Fellowship, 1993 (CSIR-UGC NET)
- National Merit Certificate by CBSE for academic excellence in AISSE, 1985

TEACHING EXPERIENCE

- 8 years at PG level

COURSES SUPERVISED AT PG Level

- ELECTROMAGNETISM
- QUANTUM STATISTICS
- ELEMENTARY SOLID STATE PHYSICS
- ADVANCED CONDENSED MATTER PHYSICS
- ATOMIC AND MOLECULAR PHYSICS
- GENERAL LABORATORY COURSE
- COMPUTER SIMULATION COURSE
- NUMERICAL METHODS IN PHYSICS – Post B. Sc. 2nd Semester S. N. Bose National Centre for Basic Sciences, Kolkata(2007 and 2008)

OTHER PROFESSIONAL ASSIGNMENTS

- Member, Women's Grievance Redressal Cell, WBSU, 2012-13

PROJECTS:

- DST-WOS(A) project, Rs. 14,00,000 (approx.), 3 years (premature termination with two months remaining after appointment at WBSU), 2006-2009

RESEARCH EXPERIENCE

More than 8 years after Ph. D. at positions equivalent to Assistant Professor

- DST WOS(A) Fellow, S. N. Bose National Centre for Basic Sciences (2006-2009)
- Visiting Faculty Fellow, S. N. Bose National Centre for Basic Sciences (2007-2009)
- Research Associate, S. N. Bose National Centre for Basic Sciences (2005-2006)
- Guest Scientist, Max-Planck Institute for Solid State Research, Stuttgart, Germany (2003-2004)
- Research Associate, IACS, Kolkata (1999-2003)

RELEVANT PUBLICATIONS

1. *Quantum chemical studies on the role of residues in calcium ion binding to Calmodulin*, S. Sikdar, M. Ghosh, **Molly De Raychaudhury**, J. Chakrabarti, Chemical Physics Letters, Volume 605-606, 103-107 (2014)
2. *Electronic structure and transport properties of early transition metal tripledeckers*, B. Das and **Molly De Raychaudhury**, Journal of Chemical Physics, Volume 134, Issue 1, pp. 014709-014710 (2011).
3. *Magnetic, optical and magneto-optical properties of PLD grown EuH₂ films*. J. Schoenes, H. Schroter, B. Lobbenmeier, **M. De Raychaudhury** and S. K. De, J. Phys.: Conference Series 200, 072087 (2010).
4. *Electronic structure of FeCr₂S₄: Evidence of Coulomb-enhanced spin-orbit splitting*, S. Sarkar, **Molly De Raychaudhury**, I. Dasgupta and T. Saha-Dasgupta **Phys. Rev. B (RAPID COMMUNICATIONS) 80**, 201101(R) (2009)
5. *Density functional study of the electronic and optical properties of the spinel compound CuIr₂S₄*, S. Sarkar, **Molly De Raychaudhury** and T. Saha-Dasgupta **Phys. Rev. B (BRIEF REPORTS) 79**, 113104 (2009)
6. *Unusual negative temperature coefficient of resistance in a crystalline solid* A. Pandey, C. Mazumdar, R. Ranganathan, **Molly De Raychaudhury**, T. Saha-Dasgupta, S. Tripathi, D. Pandey and S. Duttagupta **Euro. Phys. Lett. 84**, 47007 (2008)

7. *Moderate to large magneto-optical signals in high T_c double perovskites.*

Hena Das, **Molly De Raychaudhury** and T. Saha-Dasgupta, **Appl. Phys. Lett.** **92**, 201912 (2008)

8. *Ab-initio study of electronic, optical and magneto-optical properties of CoS_2 and $Co_{1-x}Fe_xS_2$,*

Swarup Saha, **Molly De Raychaudhury** and T. Saha-Dasgupta
Phys. Rev. B **77** 155428 (2008)

9. *Orbital fluctuations in the different phases of $LaVO_3$ and YVO_3 .*

Molly De Raychaudhury, Eva Pavarini and O. K. Andersen
Phys. Rev. Lett. **99** 126402 (2007)

10. *Ferromagnetism in metallic chalcospinels : $CuCr_2S_4$ and $CuCr_2Se_4$*

T. Saha-Dasgupta, **Molly De Raychaudhury** and D. D. Sarma
Phys. Rev. B **76** 054441 (2007)

11. *Theoretical study of doped $Tl_2Mn_2O_7$ and $Tl_2Mn_2O_7$ under pressure.*

Molly De Raychaudhury, T. Saha-Dasgupta and D. D. Sarma
Phys. Rev. B **75** 014443 (2007)

12. *Origin of ferromagnetism and its pressure and doping dependence in $Tl_2Mn_2O_7$*

T. Saha-Dasgupta, **Molly De Raychaudhury** and D. D. Sarma
Phys. Rev. Lett. **96** 087205 (2006)

13. *Electronic, optical and magneto-optical properties of Gd monopnictides: An LDA+U study*

D. B. Ghosh, **Molly De** and S. K. De
Phys. Rev. B **72** 045140 (2005)

CONFERENCE PAPERS (PEER-REVIEWED)

- *Origin of ferromagnetism in $Tl_2Mn_2O_7$ and $CuCr_2S_4$,* **Molly De Raychaudhury**, T. Saha-Dasgupta and D. D. Sarma, AIP Conference Proceedings Subseries: Materials Physics and Applications **1003** 130 (2008)

SIGNIFICANT CONFERENCE ORAL PRESENTATIONS

- “Ferromagnetism in one-dimensional TM monatomic chains with aromatic ligands”, ICFANT 2010, Jadavpur University, Kolkata, 2010
- “Chemical Route to robust ferromagnetism in monatomic transition metal chains” at CMDAYS10 held at Kalyani University, West Bengal from August 25 – 27 , 2010
- “1S-terminated surface of CoS_2 : A case of Sulphur-enriched” at CMDAYS09, held at Department of Physics, Jadavpur University, Kolkata from August 26-28th , 2009
- “Metallic Cu Chalocspinels: Ferromagnetism and related issues” at RECHARGE’08, held at S. N. B. N. C. B. S., Kolkata from 30-31 January 2008

- "Origin of ferromagnetism in pyrochlore and chalcospinels". at Workshop on Electronic Structure of Emerging Materials: Theory & Experiment, held at Lonavala, India from February 7 - 10, 2007
- "Origin of ferromagnetism and pressure and doping effects in $Tl_2Mn_2O_7$ " at SNBOSEFEST'06 held at S. N. B. N. C. B. S., Kolkata from 23-24 March, 2006

SIGNIFICANT CONFERENCE POSTER PRESENTATIONS

- Role of residues in the stability of Ca bound Calmodulin- A density functional study, Advancing Biology through Technology and Computation, 2014, WBSU
- Orbital-fluctuation induced rich electronic properties in transition metal oxides, International symposium on Recent Electronic – Structure Theories and Related experiments, http://www.fkf.mpg.de/601177/27_Poster_Session, MPI-FKF, Stuttgart, Germany, 2013
- Quantum Chemical studies on charge transfer in a metal binding loop of a protein, Current Trends in Biochemical and Biophysical Modelling, S. N. Bose National Centre for Basic Sciences, October 2013
- 3rd Indo-Japan Conference on Ferroics and Multiferroics, IACS and SNBNCBS, Kolkata from February 4-6, 2008
- Workshop on Electronic Structure of Emerging Materials: Theory & Experiment, held at Lonavala, India from February 7 - 10, 2007.
Website:<http://www.bose.res.in/workshop/talklona.htm>
- Orbital 2007, held at Max Planck Institut-FKF, Stuttgart, Germany from October 10-11, 2007
- International Conference on Magnetic Materials, SINP, Kolkata from December 11-16, 2007
- Indo-Japan Joint Seminar on Novel Giant-Magnetoresistive Materials and their Electronic Structure, held at IISc, Bangalore, India from January 29-February 2, 2006.
- Inhouse Meeting , S. N. Bose National Centre for Basic Sciences, Kolkata held at the centre on 28-29 January 2005
- Indo-US conference on Novel and Complex Materials, held at S. N. Bose Centre for Basic Sciences, Kolkata, India from October 26 - 29, 2005. Website: <http://www.bose.res.in/indous/>

SHORT VISITS

- Associate visit, S. N. Bose National Centre for Basic Sciences, 2014
- Associate visit, S. N. Bose National Centre for Basic Sciences, 2013
- Guest Scientist at Department of Earth and Environmental Sciences, Section Crystallography, Ludwig-Maximilians-University Munich, Germany on 12th October 2007
- Guest Scientist at Chair of Atomistic Modelling and Design of Materials, Department of Materials Physics, Montanuniversitat, Leoben, Austria from 13th October-17th October, 2007

OTHER INVITED TALKS (2004-2010)

- “Introduction to magneto-optical Kerr effect” at Department of Earth and Environmental Sciences, Section Crystallography, Ludwig-Maximilians-University Munich, Germany on October 12, 2007.
- “Origin of ferromagnetism in $Tl_2Mn_2O_7$ and $CuCr_2S_4$.” at Chair of Atomistic Modelling and Design of Materials, Department of Materials Physics, Montanuniversitat, Leoben, Austria on October 16, 2007.
- “Orbital fluctuations in $LaVO_3$ and YVO_3 ”, Chair of Atomistic Modelling and Design of Materials, Department of Materials Physics, Montanuniversitat, Leoben, Austria on October 17, 2007.