# Swarnakamal Mukherjee

**Assistant Professor in Physics**
**Department of Educational Science**
**Assam University Silchar**

*Curriculum Vitae*

## Personal

**Birth** : 22 August 1983
**Sex** : Male
**Nationality** : Indian

**Category** : General

**Contact No.** : +91-9474658751
**E-mail** : skphys@gmail.com

## Education

1999 **Secondary** ($10^{th}$), *West Bengal Board Of Secondary Education*, .

1999–2001 **Higher-Secondary** ($12^{th}$), *West Bengal Council of Higher Secondary Education*, .

2001–2004 **B. Sc.**, *The University of Burdwan*, ,
Physics (Hons.), Chemistry, Mathematics .

2006–2008 **M. Sc.**, *Visva-Bharati– Santiniketan* , ,
Specialized in Condensed Matter Physics .

2008 (June) **CSIR-JRF & LS (NET)**, *CSIR-HRDG* , Subject– Physical Sciences .

2009 **GATE (** **Physics** **)**, All India Rank-245, Percentile-95.50.

2009-2010 **Post-Msc**, *Satyendra Nath Bose National Centre for Basic Sciences, Block-JD, Sector-III, Salt Lake, Kolkata-700 106* .

2009 – 2017 **PhD** **Physics (Material Science)** ), *University of Calcutta*,

PhD Registration– 24/12/2012 ,
Thesis Submitted – 30/11/2015 ,
Degree Awarded– 31/01/2017 ,
Thesis Title–
Electronic Structure Of Crystallille Solids And Finite-Sized Clusters .

# Awards honours

- **NET (June, 2008)** – CSIR-JRF & Lectureship (NET)
- **GATE (2009)** – All India Rank 245 & Percentile Score 95.50

# Professional Positions

2009(Feb.)-2017(Jan.) **Junior & Senior Research Fellow**, *Satyendra Nath Bose National Centre for Basic Sciences* , *Kolkata-700 106.*

2016(Apr.)-2016(May) **Visiting Scholar**, *International Centre for Quantum and Molecular Structures* , Shanghai University.

2017(Feb.)-2017 (Oct.) **PostDoctoral Research-Associate**, *Indian Institute of Technology Kharagpur* , Kharagpur, India - 721302.

2017(Oct.)-Till Date **Assistant Professor in Physcs**, *Department of Education*, Assam University Silchar.

# Research Interests

- Electronic structure of strongly correlated systems .
- First principles investigation of Complex Oxides .
- Electronic structure and phase stability in Disordered Materials .
- Interplay between Charge, Spin and Orbital degrees of freedom .
- Magnetic anisotropy .
- Electronic structure of materials at Nanoscale and Low-Dimensional Structural composites.

# Computational Skills (proficient)

**Methods**

- Density functional theory (LDA, LSDA, GGA, GGA+U)
- Nudged Elastic Band (NEB)
- NMTO-downfolding
- Wannier basis representation

**Codes**

- VASP (https://www.vasp.at/)
- WIEN2k (http://susi.theochem.tuwien.ac.at/)
- The MTO Formalism : **LMTO** & **NMTO** (https://www2.fkf.mpg.de/andersen/docs/manual.html)

**Visualizations**

- Isosurface of Charge Density
- Wannier Functions
- Packages
  - Xcrysden :– http://www.xcrysden.org/
  - VESTA :– http://fujioizumi.verse.jp/visualization/VENUS.html
  - Data-Explorer :– http://www.data-explorer.com/

**Miscellaneous**

- fortran77 & fortran90
- Shell script
- Numerical Methods
- Latex
- Mathematica :- https://www.wolfram.com/mathematica/
- MATLAB :- https://in.mathworks.com/products/matlab.html
- Linux – MPI, LibreOffice, Gimp, Xfig, Xmgrace, gnuplot
- Windows – Microsoft Office, Photoshop, 3ds Max

# Conference Proceedings

**Talks**

- First-Principles study of $CaCu_3B_4O_{12}$ (B=Cr, Co, Rh, Ir), May-2016
  International Centre for Quantum and Molecular Structures,
  Shanghai University.
- First-Principles study of $CaCu_3B_4O_{12}$ (B=Cr, Co, Rh, Ir),
  January-2013, Bose Fest
  Satyendra Nath Bose National Centre for Basic Sciences, Kolkata-700 006
- First-Principles study of A-site ordered perovskite oxides,
  January-2014, Bose Fest
  Satyendra Nath Bose National Centre for Basic Sciences, Kolkata-700 006

**Posters**

- First-Principles study of $CaCu_3B_4O_{12}$ (B= Co, Rh, Ir), May-2012
  International Conference On Functional Oxides And New Carbon Materials,
  Satyendra Nath Bose National Centre for Basic Sciences, Kolkata-700 106.
- First Principles Investigation of Ligand-Protected Eight Atom Gold
  Nanoclusters, January-2012, Bose Fest
  Satyendra Nath Bose National Centre for Basic Sciences, Kolkata-700 006

**Attended**

- National Workshop On Condensed Matter Physics In The Last
  Decade (WCMP-2017), February-2017, Department Of Physics,
  Indian Institute of Technology Kharagpur Kharagpur, India -721302.

# List Of Publications

- **Competition between heavy fermion and Kondo interaction in isoelectronic A-site-ordered perovskites**
  D. Meyers, S. Middey, J.-G. Cheng, **Swarnakamal Mukherjee**, B.A. Gray, Yanwei Cao, J.-S. Zhou, J.B.Goodenough, Yongseong Choi, D. Haskel, J.W. Freeland, T. Saha-Dasgupta, J. Chakhalian.
  **NATURE COMMUNICATIONS, 5, 5818 (2014) .**

- **Magnetic-Structure-Stabilized Polarization in an Above-Room-Temperature Ferrimagnet**
  Man-Rong Li, Maria Retuerto, David Walker, Tapati Sarkar, Peter W. Stephens, **Swarnakamal Mukherjee**, Tanusri Saha Dasgupta, Jason P. Hodges, Mark Croft, Christoph P. Grams,Joachim Hemberger, Javier Snchez-Bentez, Ashfia Huq, Felix O. Saouma, Joon I. Jang, and Martha Greenblatt.
  **ANGEWANDTE CHEMIE INTERNATIONAL EDITION, 53, 10774 (2014).**

- **Zhang-Rice physics and anomalous copper states in A-site ordered perovskites**
  D. Meyers, **Swarnakamal Mukherjee**, J.-G. Cheng, S. Middey, J.-S. Zhou, J. B. Goodenough, B. A. Gray, J. W. Freeland, T. Saha-Dasgupta, J. Chakhalian.
  **SCIENTIFIC REPORTS 3, 1834 (2013).**

- **Polar and Magnetic $Mn_2FeMO_6$ (M=Nb, Ta) with $LiNbO_3$-type Structure: High-Pressure Synthesis.**
  Man-Rong Li, David Walker, Maria Retuerto, Tapati Sarkar, Joke Hadermann, Peter W. Stephens, Mark Croft, Alexander Ignatov, Christoph P. Grams, Joachim Hemberger, Israel Nowik, P. Shiv Halasyamani, T. Thao Tran, **Swarnakamal Mukherjee**,Tanusri Saha Dasgupta, and Martha Greenblatt.
  **ANGEWANDTE CHEMIE INTERNATIONAL EDITION, 52, 8406 (2013).**

- **First-principles study of $CaCu_3B_4O_{12}$ (B=Co, Rh, Ir)**
  **Swarnakamal Mukherjee**, Soumyajit Sarkar, T. Saha-Dasgupta
  **JOURNAL OF MATERIAL SCIENCE, 47, 7660 (2012).**

- **A first principles density functional investigation of ligand-protected eight atom gold nanoclusters.**
  Jaita Paul, **Swarnakamal Mukherjee**, Tanusri Saha-Dasgupta
  **AIP ADVANCES 1, 032150 (2011).**

- **Substantial reduction of Stone-Wales activation barrier in fullerene.**
  Mukul Kabir, **Swarnakamal Mukherjee**, Tanusri Saha-Dasgupta
  **PHYSICAL REVIEW B 84, 205404 (2011).**

# Research Experience

Scientists in this recent time are investing a lot of effort to study the physical and chemical properties of the materials. For advancement of industry, material science engineering has become a hot research topic in both theoretical and experimental fields. The vast variety of structural and physical properties exhibited by materials makes them promising for industrial applications. Material properties like structural, magnetic, optical properties primarily depend on the electrons. Study of electronic structure of materials thus forms an important area in condensed matter science. Advancement in technique like density functional theory (DFT), makes the theoretical study of electronic structure effcient. During past decades, computational material science has emerged as one of the important field of research. Designing new materials with unique properties from the ab initio calculations using the electronic structure methods is one of the exciting and interesting areas of theoretical research. Nowadays, with the availability of fast computers and efficient algorithm, first principles electronic structure calculation has emerged as an effective tool to design 'novel materials' with novel properties.

In this context, transition metal oxides are one of the most interesting class of crystalline solids, exhibiting wide-ranging varieties in crystal structures and electronic properties. Properties exhibited by the transition metal compounds depend on the quantum cloud of the d electrons, bonding nature between transition metal and oxygen. Charge-orbital interplay existing in such compounds results in high $T_C$ superconductivity in layered cuprates, colossal magneto resistance (CMR) in perovskite manganites, coexistence of magnetism and ferroelectricity - termed as multiferroicity, coexistence of magnetism and superconductivity in heavy fermion systems, quantum phase transitions to name a few. Electron-electron correlation has a dominant contribution to the ground state properties of such transition metal compounds. In the limit of strong electronelectron correlation, localized electrons describe the Mott insulating state characterized by the anti-ferromagnetic spin ordering. In addition to the Mott-Hubbard electronelectron correlations, the relativistic effect and the ligand field effect are also important aspects of the transition metal based compounds. The relativistic correction gives rise to the so-called spin-orbit interaction which becomes important for "heavy" transition metal. Different ligand field makes different d orbitals being responsible for the bonding. Crystal field dominated orbital physics forms an important component for the first-principle electronic structure studies.

In addition to the crystalline solids, first principle based simulations have been also very successful in describing the electronic structure of materials at nano-meter length scale, an important topic for both science and engineering. Quantum confinement effect plays a crucial role for such low dimensional materials. In this category, nanoclusters are systems of profound research interest since they offer applications in various fields such as nanocatalysis, biomedical sciences and in nanotechnology industry in general. Though several investigations have been conducted to understand the properties of these clusters, several challenges still remain. It is well known that the properties of clusters not only deviate significantly from their bulk behavior but they also exhibit strong dependence on the size and the atomic arrangement of the cluster. This in turn affects the nature of the bonds formed when these clusters interact with other compounds as often is the case when they are used in *e.g.*, catalysis. Detailed understanding of the structural evolution of nanoclusters and their electronic properties is thus extremely important.

**Quadruple Perovskite – $CaCu_3B_4O_{12}$ (B=Cr, Co, Rh, Ir) :–**

Here we perform electronic structure calculations on A-site-ordered perovskites with Cu in the A-site and the B-sites descending along the ninth group of the periodic table to elucidate the emerging properties as $d$-orbitals change from partially filled $3d$ to $4d$ to $5d$. The results show that when descending from $3d$ to $4d$ to $5d$, the charge transfers from the cuprate-like Zhang-Rice state ($d^8\underline{L}$, $\underline{L}$ denotes an oxygen hole) on Cu to the $t_{2g}$ orbital of the B site. In low dimensional cuprates several interesting phenomena, including high $T_c$ superconductivity, are deeply connected to electron correlations on Cu and the presence of this Zhang-Rice (ZR) singlet state. As the Cu $d$-orbital occupation approaches the Cu-$2p$ limit, a mixed valence state in $CaCu_3Rh_4O_{12}$ and heavy fermion state in $CaCu_3Ir_4O_{12}$ are obtained. The investigated $d$-electron compounds are mapped onto the Doniach phase diagram of the competing RKKY and Kondo interactions developed for the $f$-electron systems.

**Corundum Derivatives – Polar Oxides :–**

Recently, exotic $ABO_3$-type perovskites with unusually small A-site cations have attracted much attention owing to the formation of polar structure at high pressure. The crystal structure of corundum-type oxides consists of hexagonal close packing of the oxygen atoms, where the metal atoms occupy two-thirds of the octahedral sites, the remaining one-third of the octahedral sites are vacant. Given the same corundum-type rhombohedral stacking of octahedra, different crystal structures can be derived, including $ABO_3$-type ilmenite (IL), $LiNbO_3$ (LN) and $A_2BB'O_6$-type ordered IL, $Ni_3TeO_6$ structures. Polar $Mn_2{}^{2+}Fe^{3+}M^{5+}O_6$ (M=Nb, Ta) show LN-type ($R3c$) structures while non-centrosymmetric ($R3$) $Ni_3TeO_6$ phase of $Mn_2{}^{2+}Fe^{3+}M^{5+}O_6$ (M=Mo) becomes energetically favourable. $Mn_2{}^{2+}Fe^{3+}Mo^{5+}O_6$ demonstrates structural polarization without any ions with $(n-1)d^{10}ns^0$, $d^0$ or stereoactive lonepair electrons. The crystal structure of $Mn_2{}^{2+}Fe^{3+}Mo^{5+}O_6$ breaks the polarization rule, because known polar perovskite-related and corundum-based compounds contain ions with either $(n-1)d^{10}ns^0$ or $d^0$ electronic configuration. $Mn_2{}^{2+}Fe^{3+}Mo^{5+}O_6$ is the first example where noncentrosymmetric structure and spontaneous polarization can be stabilized in a corundum-based compound that orders ferrimagnetically above room temperature.

**$C_{60}$ – Stone-Wales (SW) activation barrier :–**

Stone-Wales (SW) activation barrier for $I_h$-$C_{60}$ formation is very high ($\sim$ 5.3 eV). This large barrier height can be reduced in presence of extra carbon atom. The growth of fullerene results from the autocatalysis by such loosely bound carbon atoms. We have shown that substitutional doping at the SW sites is a much more effective route for such mechanism. Our calculations reveal that presence of a single boron at the active SW site reduces this activation barrier by an amount of $\sim$ 2.2 eV, while company of another boron at the nearest SW active site minimize this energy cost to $\sim$ 0.76 eV which is the minimum value of the SW activation energy barrier reported till date.

**$Au_8$ – Ligation effect on Gold Nano-structures :–**

The properties exhibited by the gold clusters are found to be extremely sensitive to the size, structure and dimension of the cluster. Gold clusters are reported to retain their planar structures to cluster sizes larger compared to Ag and Cu clusters due to the strong sd-hybridization which is purely relativistic effect. Here we investigate the effect of ligand capping on the results of the earlier studies on the stabilization of 2D and 3D geometries. 8-atom Au clusters was a suggested number for a probable 2D-3D transition for bare clusters and it has been synthesized experimentally. Ligation enhances the stability of 2D geometry over non-planner structures.

# Orientatition Programme

- *115th Orientation Programme at U.G.C.- HUMAN RESOURCE DEVELOPMENT CENTRE, The University of Burdwan ( 08/08/2019 to 28/08/2019)*

# Research Project

- " Electronic structure in correlated electronic systems " Funded by UGC ( **UGC Start-Up Grant**). (2019 - 2022).



Swarnakamal Mukherjee
Department of Education - Assam University Silchar

+91-9474658751 • ✉ skphys@gmail.com