Senior Research Fellow specializing in quantum transport across magnetic tunnel junctions (MTJ) with transition metal impurities in the insulating barrier. Transport is studied using the Non-equilibrium Green's function method within the tight binding model and the impurities are described using the Single Impurity Anderson Model. In the process of developing a phenomenological model that can be used to obtain transport characteristics of any given MTJ with random transition metal impurities in the barrier and other functionalities of importance in MRAMs like spin transfer torque and switching efficiencies.

PARVATHY HARIKUMAR

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Languages

English
Tamil
Hindi
Malayalam

Experience 2016-2023

- **Expertise in FORTRAN programming and an intermediate level knowledge with hands-on-experience in Python coding**
- **Knowledge of numerical methods to implement transport using tight binding method, dynamical mean field theory models to describe partially filled TM impurities and strongly correlated materials.**
- **Hands-on experience in Density functional theory(DFT) packages like VASP and Wannier90 using VASP interface**
- **Theoretical understanding and FORTRAN code implementation of Non-equilibrium Green's function (NEGF) formulation to electronic transport in tunnel junctions**
- **Combining *ab-initio* methods like DFT with theoretical models to obtain effective positions of impurity states in typical 3D and 2D insulators like Aluminum Nitride (AlN) , Graphene etc.**
- **Writing and implementing FORTRAN codes to study spin transfer torque in model tunnel junctions**
- **Multiband generalization of NEGF formulation to include tight binding parameters fitted to realistic electronic band structure of 2D materials/hetero-structures (VN-AlN)**
- **Basic knowledge of Slater-Koster tight binding (TB) method and its application to fitting of TB parameters for bulk materials such as cubic VN and wurtzite AlN**
- **Coding knowledge in Python for application to materials science as implemented in packages like Transiesta for transport calculations using DFT-TB methods.**
- **Basic knowledge in calculation of material properties using Quantum Espresso**

Education 2010-2023

Doctor of Philosophy (Ph.D.): Physics (pursuing), Computational Materials Science, Indira Gandhi Center for Atomic Research (IGCAR), Kalpakkam, Tamil Nadu, India (Completed)

Master of Science: Physics, Theoretical Physics department, University of Madras, Tamil Nadu, India

Bachelor of Science: Physics, Madras Christian College, Tambaram, Tamil Nadu, India

Skills

Software:

- **Expertise in C++ and FORTRAN programming**
- **3+ years of experience in 2D and 3D materials/hetero-structure modeling in latest VASP packages**
- **Expertise in documentation using LaTeX software and plotting softwares such as XmGrace, Origin etc.**
- **5+ years of experience in FORTRAN code development and compilation to study complex physical phenomena**
- **Intermediate programming skill in Python for machine learning**
- **Beginner level hands-on-experience in Quantum Espresso and SIESTA packages.**

Professional:

- **Excellent written and oral communication skills and the ability to communicate to an international, scientific audience**
- **Motivated self-starter with the ability to work independently and to participate creatively in collaborative teams across the laboratory**
- **Ability to function well in a fast-paced research environment, set priorities to accomplish multiple tasks within deadlines, and adapt to ever changing needs**
- **Proven record of productive and creative research as demonstrated by publications in peer-reviewed journals**

Conferences/ Workshops

1. Magnetoresistance of tunnel junctions containing Anderson impurities, Parvathy Harikumar, S Mathi Jaya, 2*nd* Indian Materials Conclave and 31*st* AGM, Materials Research Society, Feb 11-14 (2020), Kolkata

2. Magnetic and electronic properties of transition metal doped Aluminium Nitride: Haldane's approach combined with ab initio results, Parvathy Harikumar, S Mathi Jaya, Sharat Chandra, 65*th* annual conference on Magnetism and Magnetic Materials (Virtual conference), Florida, United States, Nov 2-6, (2020)

3. Online Hands-on workshop with TBtrans, TranSiesta and SISL, practice of DFT-TB parametrization in CECAM flagship school on "Advanced school on quantum transport using SIESTA", Spain, May 17-21 (2021)

4. Effect of interaction strength on magnetic properties of transition metal doped hexagonal Aluminum Nitride monolayer, Parvathy Harikumar, Sharat Chandra, DAE-SSPS (Virtual conference), Mumbai, Dec 15-19 (2021)

Publications

1. **Non-equilibrium Green's function modeling of the transport characteristics of magnetic tunnel junctions containing Anderson impurities, Parvathy Harikumar, S Mathi Jaya, SPIN, 10, 2050006,(2020)**
2. **Magnetic and electronic properties of transition metal doped Aluminium Nitride: Haldane's approach combined with ab initio results, Parvathy Harikumar, S Mathi Jaya, Sharat Chandra, AIP Advances 11, 035222 (2021)**
3. **Enhanced spin transfer torque in single barrier model tunnel junctions containing disordered interface, Parvathy Harikumar and Sharat Chandra, SPIN 12, 9 (2022)**
4. **Interface structure and bias dependence of VN/AlN/VN tunnel junction: A semi-empirical calculation, Parvathy Harikumar, Mayank Gupta, R. K. Nanda, Sharat Chandra, Journal of Magnetism and Magnetic Materials Vol. 586, No. 15, 171191 (2023)**