Simran **Kumari**

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Education

University of California
Los Angeles, California

Graduate School, Chemical Engineering — *Sept. 2019 - Present*

- Cumulative GPA : 4/4

Indian Institute of Science Education and Research
Kolkata, India

Master of Science - Chemistry — *July 2016 - May 2018*

- Cumulative GPA : 8.9/10

Indian Institute of Science Education and Research
Kolkata, India

Bachelor of Science - Chemistry — *July 2013 - May 2015*

- Cumulative GPA : 8.9/10

Research Experience

University of California, Los Angeles (UCLA)
Los Angeles, California

Graduate Student under **Prof. Philippe Sautet**. (Sautet Lab at UCLA) — *Sept. 2019 - Present*

- Multi scale modeling of Pt-clusters on supports for electrocatalysis.
- Studying the electrochemistry of different Pt clusters-Ptn(n = 1,2,3,8) on Indium oxide and Indium Tin oxide supports.
- Finding the best adsorption site and structure for the cluster using Grand Canonical Basin Hopping.
- Introducing explicit water to study the interaction of water/hydroxyl molecules on the adsorption of the clusters.
- Introducing implicit solvation and studying the catalyst/electrolyte interface using linear Poisson-Boltzman equation at different electrolyte charge.
- Using the Computational Hydrogen Electrode to understand the Hydrogen Evolution Reaction and the electrocatalytic capabilities of the system.

École Polytechnique Fédérale de Lausanne (EPFL)
Lausanne, Switzerland

Master's student under **Prof. Nicola Marzari**. (Theory and Simulation of Materials) — *Dec. 2017 - Sept. 2019*

- Superconductivity in 24 layered materials.
- Performing electron-phonon calculations using Wannier interpolation through EPW/Quantum ESPRESSO on different types of 2D materials to find potential high-T_c superconductors.
- Effects of doping and strain in the systems with the highest T_c.

Indian Institute of Science Education and Research (IISER-Kolkata)
Kolkata, India

Undergraduate student with **Dr. Ashwani Kumar Tiwari**. — *May 2017*

- Studying NiCo-based oxide and oxysulfide materials for OER and understanding the advantages of using metal oxysulfides over their oxide counterparts.
- Studying the electrochemical capabilities of $NiCo_2O_xS_{4-x}$ and $NiCo_2O_4$ using Oxygen Evolution Reaction.
- Understanding the significance of Sulphur on the increased catalytic activity of $NiCo_2O_xS_{4-x}$ when compared to $NiCo_2O_4$ by comparing the electronic properties such as Density of States and utilizing the p/d-band theory.

Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)
Bangalore, India

Visiting Student under **Prof. Umesh V. Waghmare**. — *Summers 2016*

- First-principles study of h-BN/graphene and 2H/1T-MoS_2 heterostructures.
- Studied the structural and electronic effects of h-BN/graphene on 2H-MoS_2/1T-MoS_2 monolayers.
- Constructed heterostructures of 2H/1T-MoS_2 and h-BN/graphene with minimum lattice mismatch and performed first-principles calculations based on density functional theory (DFT).
- Examined the structural distortions created by hBN/graphene on 1T-MoS_2 and studied its co-relation with the change in the electronic structure of 1T/2H MoS_2(opening up of a band-gap in 1T-MoS_2).

National Chemical Laboratory (NCL) *Pune, India*

Summer research fellow under **Dr. Suman Chakrabarty**. *2014-2015*

- Studied Protein misfolding and aggregation.
- Simulated system of prions using Molecular Dynamics methods implemented in GROMACS.
- Employed the technique of REMD(Replica Exchange Molecular Dynamics) to enhance the sampling and to explore new conformations space
- Performed secondary structure analysis using DSSP and other analysis were done using the in-house tools in GROMACS to find RMSF, minimum distance vs residue between the two prions and the frequency of Hydrogen bonding between the prions.

Bhabha Atomic Research Centre (BARC) *Mumbai, India*

NIUS fellow under **Dr. MAHESH SUNDARARAJAN.**. *2014*

- Studied Nitrite-Nitrito Linkage Isomerism in Manganese mutated Myoglobin.
- Studied the dependence of energy of the optimized structure of different spin states (Low spin, Intermediate Spin and High spin.) on functionals such as BP86 and B3LYP.
- The calculations were done using TURBOMOLE and single point energy calculations were done using ORCA.
- The initial structures of Fe-Mb, Co-Mb and MN-Mb where taken from the Protein Data Bank. Contrasted a Big Model (with His64) and a small model (without His64) to understand the significance of His64 in Nitrate binding.

Academic Projects

Voluntary Undergraduate Researcher under **Prof. Pradip Kumar Ghorai** *Semester 3*

- Worked on a reverse micelle system and performed simulations using Molecular Dynamics as implemented in the DL-POLY package.
- Built a system of reverse micelles immersed in water and studied its dynamics.

Voluntary Undergraduate Researcher under **Prof. Raja Shunmugam** *Semester 4*

- Worked in the field of polymer chemistry. Learned different techniques to synthesize and characterize monomers and polymers.
- Free radical growth polymerization (bulk, suspension and emulsion) of styrene, anionic polymerizatoin and cationic polymerization of MMA and styrene.
- Used characterization techniques such as IR and 1H-NMR.

Publications

- Davide Campi, **Simran Kumari** and Nicola Marzari "Prediction of phonon-mediated superconductivity with high critical temperature in the two-dimensional topological semimetal W_2N_3." Accepted Manuscript - Nano Letters
- **Simran Kumari** and Ashwani K. tiwari, (2018) "H_2 dissociation on differently shaped Ni patches on Pt (111) surface.", *manuscript in preparation*.
- Ahmed, Tanweer, Mit H. Naik, **Simran Kumari**, Smriti P. Suman, Rahul Debnath, Sudipta Dutta, Umesh V. Waghmare, Manish Jain, and Arindam Ghosh. "Thermodynamically stable octahedral MoS2 in van der Waals hetero-bilayers." 2D Materials 6, no. 4 (2019): 041002.
- Sagar Ganguli, Soumik Das, **Simran Kumari**, Harish Reddy Inta, Ashwani Kumar Tiwari, and Venkataramanan Mahalingam. "Effect of Intrinsic Properties of Anions on the Electrocatalytic Activity of $NiCo_2O_4$ and $NiCo_2O_xS_{4-x}$ Grown by Chemical Bath Deposition." ACS Omega 3, no. 8 (2018): 9066-9074.

Skills & Techniques

- Proficient in performing **Molecular Dynamics** and **Density Functional Theory** simulations.
- Experience working with **VASP,Gromacs, Turbomole, Gaussian, DL-POLY, ORCA and Quantum ESPRESSO** for simulating/optimizing the structures and studying its chemical/physical properties.
- Comfortable with programming languages such as **Python, FORTRAN, and LaTeX**.
- Comfortable with Python frameworks such as **PANDAS, SciKit-Learn, Numpy, Matplotlib**.
- Worked with various visualization softwares including **Chimera, ChemDraw, GaussView, Molden, VMD, Materials Studio** and **Xcrysden**.
- Experience with plotting libraries/software such as **Gnuplot, Qtiplot and xmgrace**.
- Comfortable with **Bash**, having used it frequently for the post processing of computational results.
- Using **MPI and high-performance computing** on a regular basis to conduct my research work.