Simran **Kumari**

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Education

University of California	*Los Angeles, California*
PH.D., CHEMICAL ENGINEERING	*Sept. 2019 - June 2023*

- GPA : 4/4

Indian Institute of Science Education and Research	*Kolkata, India*
BACHELORS AND MASTERS OF SCIENCE - CHEMISTRY	*July 2013 - May 2018*

- GPA : 8.9/10

Industry Experience

Nissan North America, Inc.	*Santa Clara, CA*
RESEARCH SCIENTIST	*July 2023 - Present*

- Developed novel Physics-Informed ML models for battery end-of-life prediction. Designed various differential capacity (dQ/dV) curves based features and physics-informed loss functions, achieving a MAE of 0.59%.
- Developed an ML model to predict inter-atomic potentials, using it for high-fidelity simulations of solid-state battery cathode materials. Identified multiple novel Ni and Co-free cathode materials with high energy density.
- Developed a Gaussian Process Regression (GPR) model to predict the redox potential and quenching abilities of additive molecules. Identified a set of additives that moved the thermal runaway temperature of NMC based Li-ion batteries by 15%

Nissan North America, Inc.	*Santa Clara, CA*
RESEARCH INTERN	*Feb. 2022 - Jan 2023*

- Conducted full-scale reaction mechanism studies to investigate how additives influence electrolyte interactions, aiming to reduce cathode degradation. Optimized chemical stability by understanding the degradation pathways, providing insights for enhancing cathode longevity.
- Utilized pre-trained ML inter-atomic potential models for high-throughput studies to identify new halide-based solid-state electrolytes with the lowest heat generation, enhancing battery safety and performance.

Schrödinger, Inc	*New York, NY*
MATERIAL SCIENCE INTERN	*Aug. 2021 - Feb. 2022*

- Contributed to the development and implementation of automated workflows within the Schrödinger software suite, focusing on thermodynamic and kinetic simulations for heterogeneous catalysis studies.
- Designed and tested automated workflows for CO_2 reduction on various transition metals, streamlining the evaluation process for C_1 product formation.
- Developed methodologies for generating images of Nudged Elastic Band (NEB) simulations, enhancing the visualization and analysis capabilities for studying transition states and minimum energy paths in reaction mechanims.

Research Experience

University of California, Los Angeles (UCLA)	*Los Angeles, California*
GRADUATE STUDENT UNDER **PROF. PHILIPPE SAUTET**. (Sautet Lab at UCLA)	*Sept. 2019 - July 2023*

- Focused on the development of energy materials for CO_2 reduction and hydrogen production, targeting sustainable solutions to mitigate climate change.
- Investigated the mechanisms of Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER) on Pt-doped Indium Tin Oxide (ITO) surfaces, utilizing Density Functional Theory (DFT) and microkinetic modeling to reveal key factors affecting catalytic activity. The catalyst was found to be more electrochmically active than the state-of-art Pt/C catalysts for H_2 production.
- Employed Grand Canonical Basin Hopping (GCBH) algorithms to identify the most stable configurations of active sites on catalyst surfaces, accounting for variable adsorbate coverage and experimental conditions. Tuning the coverage and experimental conditions lead to increased catalytic activity.
- Applied GCBH and DFT to study CO_2 hydrogenation on ZrO_2-Cu surfaces, optimizing reaction conditions and elucidating the role of hydroxyl groups and formates in enhancing catalytic performance for $CO2_2$ hydrogenation to value added products.

École Polytechnique Fédérale de Lausanne (EPFL) *Lausanne, Switzerland*

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

- Conducted high-throughput simulations to study superconductivity in 24 layered materials using advanced quantum mechanical methods.
- Developed and implemented automated workflows for electron-phonon calculations to accelerate the discovery of potential high-temperature superconductors.
- Performed detailed studies on the physical properties of various 2D materials using Wannier interpolation with EPW/Quantum ESPRESSO, focusing on electron-phonon coupling.
- Identified the highest-Tc superconductor for any 2D material through systematic computational screening.

Publications

- Kümper, Justus, Sonja D. Mürtz, Yani Guan, **Simran Kumari**, Peter JC Hausoul, Nils Kurig, Philippe Sautet, and Regina Palkovits. "Metallic Impurities in Electrolysis: Catalytic Effect of Pb Traces in Reductive Amination and Acetone Reduction." Angewandte Chemie: e202411532.
- Guan, Yani, Justus Kümper, Sonja D. Mürtz, **Simran Kumari**, Peter JC Hausoul, Regina Palkovits, and Philippe Sautet. "Origin of copper dissolution under electrocatalytic reduction conditions involving amines." Chemical Science (2024).
- **Simran Kumari**, Anastassia N. Alexandrova, and Philippe Sautet "Nature of Zirconia on a Copper Inverse Catalyst Under CO_2 Hydrogenation Conditions" J. Am. Chem. Soc. 2023, 145, 48, 26350–26362
- **Simran Kumari** and Philippe Sautet "Elucidation of Active site for Oxygen Evolution Reaction on Highly Dispersed Single Atom Pt Supported on indium tin oxide." J. Phys. Chem. Lett. 2023, 14, 10, 2635–2643
- Kangze Shen, **Simran Kumari**, Yu-Chao Huang, Joonbaek Jang, Philippe Sautet and Carlos G. Morales-Guio "Electrochemical Oxidation of Methane to Methanol on Electrodeposited Transition Metal Oxides" J. Am. Chem. Soc., DOI : 10.1021/jacs.3c00441
- **Simran Kumari**, Tsugonosuke Masubuchi, Henry Sheldon White, Anastassia Alexandrova, Scott L Anderson, Philippe Sautet "Electrocatalytic hydrogen evolution at full atomic utilization over ITO-supported sub-nano Ptn clusters: High, size-dependent activity controlled by fluxional Pt hydride species" J. Am. Chem. Soc. 2023, 145, 10, 5834–5845
- **Simran Kumari** and Philippe Sautet "Highly dispersed Pt atoms and clusters on hydroxylated indium tin oxide: A view from first-principles calculations." J. Mater. Chem. A, 2021, 9, 15724-15733
- Xiaoyang Fu, Dongfang Cheng, Chengzhang Wan, **Simran Kumari**, Hongtu Zhang, Ao Zhang, Huaixun Huyan, Jingxuan Zhou, Huaying Ren, Sibo Wang, Zipeng Zhao, Xun Zhao, Jun Chen, Xiaoqing Pan, Philippe Sautet,Yu Huang, Xiangfeng Duan "Bi-functional ultrathin RhRu0.5 alloy nanowire electrocatalysts for hydrazine assisted water splitting." Advanced Materials, DOI : 10.1002/adma.202301533
- 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." Nano Lett. 2021, 21, 8, 3435–3442
- 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

- **Advanced Simulation Techniques**: Proficient in Molecular Dynamics (MD) and Density Functional Theory (DFT) simulations for analyzing material properties and catalytic mechanisms.
- **Machine Learning and Data Analysis**: Proficient with machine learning frameworks such as PyTorch, as well as Python libraries like Pandas, SciKit-Learn, NumPy, and Matplotlib for data processing, model development, and scientific visualization.
- **Programming and Scripting**: Skilled in Python, FORTRAN, and LaTeX for developing computational workflows, automating simulations, and performing data analysis.
- **Computational Chemistry Software**: Extensive experience with VASP, Gromacs, Turbomole, Gaussian, DL-POLY, ORCA, and Quantum ESPRESSO for structure optimization, electronic structure calculations, and dynamic simulations.

Achievements

2021	Selected for the **DE Shaw Research Graduate and Postdoc Womens's Fellowship.**	*New York, USA*
2019	Selected for the **UCLA CBE department scholarship.**	*Los Angeles, USA*
2017	Selected for the **INSPIRE Potentials – NCCR MARVEL Master's Fellowships.**	*EPFL, Lausanne*
2014	Selected as a **National Initiative on Undergraduate Science (NIUS) fellow.**	*Mumbai, India*
2013	Recipient of **'INSPIRE' scholarship** awarded to the **top 1% of students** of India.	