Utkarsh Singh

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A research enthusiast, seeking a PhD position for fall 2019

Areas of Interest

Multifunctional Materials, First-principle Calculations, Molecular Simulations, Mathematical Modelling

Academic Details

2015 – Present **Bachelors of Technology, Chemical Engineering**.
Indian Institute of Technology, Roorkee, India
GPA: 7.95 on a 10.00 point scale (Upto 6 semesters)

2012 – 2014 **Senior Secondary Education**.
Central Board of Secondary Education, India
92.8%

2010 – 2012 **Secondary Education**.
Central Board of Secondary Education, India
GPA: 10.00 on a 10.00 point scale

Internships

May – July 2018 **Exploring Phase Stability and Magnetism in Full-Heusler Alloys**.
CRANN, Trinity College Dublin, Ireland - Prof. Stefano Sanvito
Carried out Electronic Structure Calculations, at the level of Density Functional Theory, for alternative crystal structures and possible complex magnetic ground states. In a significant number of cases, especially for Unconventional Heuslers, was able to identify new lowest energy structure below the convex hull diagram for given chemical composition. *–VASP (DFT), Statistical Physics*

May – July 2017 **Investigating 2-Dimensional Borophene sheets on intermetallic substrates**.
Vijay Kumar Foundation, India - Dr. Vijay Kumar (previously IMR, Tohoku University)
Investigated the electronic and structural properties of a variety of 2-D Borophene sheets on differnt suitable intermetallic substrates using Electronic Strucure Calculations via. DFT approach. Currently working on a manuscript to be published in a reputed peer-reviewed journal. *–VASP (DFT)*

Computer skills

Packages VASP, GROMACS, FPLO®, Quantum Espresso, Wien2k, , Linux

Languages C++, Python, Bash Scripting, MATLAB, LaTeX, HTML, CSS, JavaScript

Research Projects

August, 2018 – Ongoing **Multiscale Modelling of Polymeric Systems (Final year project)**.
Department of Chemical Engineering, IIT Roorkee - Dr. Prateek Kumar Jha
As part of my final year project, I'm working on investigating Aggregation of a polymeric system as a function of pH level of the system via. systematic course graining using the results of Atomistic level simulations. *–GROMACS (MD), Systematic Course Graining*

September, 2018 – Ongoing **Alkali metal based Alloys as High F.O.M. thermoelectrics**.
Department of Chemistry, IIT Roorkee - Dr. Hem Chandra Kandpal
Thermoelectric investigation of Alkali metal based **Heuslers** where we use Wien2k, BoltzTraP and Phono3py (with VASP) to calculate electronic, transport and thermal properties respectively.
– *Wien2k, BoltzTraP, Phono3py, VASP*

January – April 2018 **CFD modelling of a PCR reaction using COMSOL-Multiphysics (Course)**.
Department of Chemical Engineering, IIT Roorkee - Dr. Prateek Kumar Jha
With the aim to explore the use and functioning of Microreactors in Diagnostic applications as part of the Process modelling and Simulation Course, one of which is in a PCR unit, whose function is to divide and then Multiply DNA from blood samples. Used COMSOL to model the mass transfer & momentum and three stages of PCR. – *COMSOL Multiphysics*

July – September 2017 **Design of effecient materials for Photocatalytic Water Splitting** .
Department of Chemistry, IIT Roorkee - Dr. Hem Chandra Kandpal
Our collaborators at IISER Mohali, India identified a stable 'Ta' based material whose efficiency for OER compares to some of the best materials reported for Water splitting. Our job was to explain this on the basis of properties derived from the bandstructure of the material. – *Wien2k*

Community Service

Volunteer, Rural Education Cell, National Service Scheme (NSS)- IITR.
Through this initiative, students in their freshman year teach young kids from surrounding villages who can't afford tutors and are lacking in basics or, are appearing for High-school examinations.

Special Interest Group.
This is a small group some of us like minded people started to promote research among undergrads. Common activities include lectures form peers on informative topics and industrial problem-solving ranging from *Working of a mosquito repellent machine* to *How crypto-currency works.*

Extra-Curriculars

2018 – Present **Undergraduate Teaching Assistant**.
Physcial Chemistry (CY-001) - IIT Roorkee

2017 – 2018 **General Secratary** .
Indian Institute of Chemical Engineers (IIChE) Students' Chapter - IIT Roorkee

2015 – 2017 **Editor**.
Watch Out! - Student Media Body - IIT Roorkee

Languages

Hindi Native Speaker

English Fluent *language used throughout formal education*

References

Dr. Stefano Sanvito
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Head, Vijay Kumar Foundation
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Hobbies and Interests

- Reading, Tennis, Web-Design, Writing