Utkarsh Singh

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I'm interested in Materials & seeking a PhD position for fall 2020

Areas of Interest

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

Academic Details

2015 – 2019 **Indian Institute of Technology, Roorkee, India**.
Bachelors of Technology, Chemical Engineering
GPA: 7.89 on a 10.00 point scale

2012 – 2014 **Central Board of Secondary Education, India**.
Senior Secondary Education
95.4%

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

Publications

2020 *Research Article* – **Ultralow thermal conductivity owing to favourable lattice dynamics in Alkali metal based Full - Heusler Alloys (To be communicated soon)**.
Utkarsh Singh, Mohd. Zeeshan, Jeroen van den Brink and Hem C. Kandpal

2019 *Research Article* – **First-principles investigations of orthorhombic-cubic phase transition and its effect on thermoelectric properties in cobalt-based ternary alloys**.
Sapna Singh, Mohd. Zeeshan, **Utkarsh Singh**, Jeroen van den Brink and Hem C. Kandpal, *J. Phys.: Condens. Matter* **32** 055505, Nov. 2019

2020 *Software* – ***convex* – Create phase diagrams via Convex-hull approach**.
Utkarsh Singh, Github Repo. DOI: 10.5281/zenodo.3693036

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 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 polymorphs 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, FPLO®, Quantum Espresso, Wien2k, UNIX

Languages Python, C/C++, bash scripting, MATLAB, LaTeX, HTML, CSS, JavaScript

Research & Course Projects

Dec. 2018 – Jan. 2020 **Ultralow thermal conductivity owing to favourable lattice dynamics in Alkali metal based Full-Heusler alloys**.
Department of Chemistry, IIT Roorkee - Dr. Hem Chandra Kandpal
Significantly low thermal conductivity in soft, Alkali-metal based ternaries was found by *first-principles* calculations (VASP). Investigated various aspects of phonon transport (phono3py) and lattice dynamics (COHP) as the cause of such. Was able to successfully explain the origin of low thermal conductivity in the systems in focus. Also calculated thermoelectric properties. (EPW, BoltzTraP2) – *VASP (DFT), Electron-phonon Wannier, phono3py, BoltzTraP2*

August – September 2019 **Thermodynamic stability of Cobalt - based ternary alloys undergoing phase - transition**.
Department of Chemistry, IIT Roorkee - Dr. Hem Chandra Kandpal
Calculated the thermodynamic stability of multiple Co - based alloys before and after pressure - induced transition between orthorhombic and cubic phases. This was performed with a python code I wrote myself and with the help of Materials databases. – *Python, VASP (DFT)*

January – April 2018 **CFD modelling of a PCR reaction using COMSOL Multiphysics**.
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*

Extra-Curriculars

2018 – 2019 **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; TOEFL – 112/120 *language used throughout formal education*

References

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Dr. Stefano Sanvito
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Interests

- Chess, Tennis, Web-Design