

# Dr. Kumar Sonu

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## OBJECTIVE:

Designing key materials for chemical reactions and energy related processes using computations based on density functional theory and beyond is broad topic of my research. I combine theory, computations, and machine learning to design atomic structures for catalytic and energy applications.

## WORK EXPERIENCE:

**Mitsui Chemicals Postdoc:** ICReDD, Hokkaido University, Japan [July 2023 to Feb 2025]

**CREST Postdoc:** Chemistry Department, Hokkaido University, Japan [July 2022 - July 2023]

**WPI Postdoc:** ICReDD, Hokkaido University, Japan [July 2019 - July 2022]

**Postdoc:** MRC, IISc Bangalore, India [Jan 2018-June 2019]

**Guest Faculty:** CUHP, India [July 2017-Dec 2017]

**Postdoc:** PSE division, [KAUST](https://www.kaust.edu.sa/), Saudi Arabia [Feb 2014 - April 2017]

## EDUCATION:

- **Indian Institute of Technology (IITD), PhD degree, INDIA** (Aug 2008 – Nov 2013)
- **Panjab University, M.Sc. Physics (Hons School)** (2006)
- **Himachal Pradesh University, B.Sc. pass courses in Physics, Chemistry, and Math** (2004)
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## KEY PUBLICATIONS:

- **Sonu Kumar**, Karan Deep, Shagun Nag, Ranjan Kumar, "Connecting dielectric response to dominant vibrations and tolerance factors in pyrochlore oxides", **Materials Today Communications**, 38, 108415 (2024).
- Koki Ogawara, Osamu Inanami, Hideo Takakura, Kenichiro Saita, Kohei Nakajima, **Sonu Kumar**, Naoya Ieda, Masato Kobayashi, Tetsuya Taketsugu, Mikako Ogawa, "Theoretical Design and Synthesis of Caged Compounds Using X-Ray-Triggered Azo Bond Cleavage", **Advanced Science**, 2306586 (2024).
- **Sonu Kumar**, Andrey Lyalin, Zhenguo Huang, Tetsuya Taketsugu, "Catalytic Oxidative Dehydrogenation of Light Alkanes over Oxygen Functionalized Hexagonal Boron Nitride", **ChemistrySelect**, 7 (2022) e202103795.
- Sapajan Ibragimov, Andrey Lyalin, **Sonu Kumar**, Yuriko Ono, Tetsuya Taketsugu, Maciej Bobrowski, "Theoretical design of nanocatalysts based on (Fe<sub>2</sub>O<sub>3</sub>)<sub>n</sub> clusters for hydrogen production from ammonia", **Journal Chemical Physics**, 162, 054305 (2025)
- S. Sharma\*, **S. Kumar\*** and U. Schwingenschlögl, Arsenene and antimonene: Two-dimensional materials with high thermoelectric figures of merit, **Phys Rev Applied**, 8 (2017) 044013
- **S. Kumar** and U. Schwingenschlögl, Thermoelectric performance of functionalized Sc<sub>2</sub>C MXenes, **Phys. Rev B**, 94 (2016) 035405.