Hena Das Lab.

Theoretical and Computational Materials Physics:

Investigations and Prediction of quantum phenomena in materials

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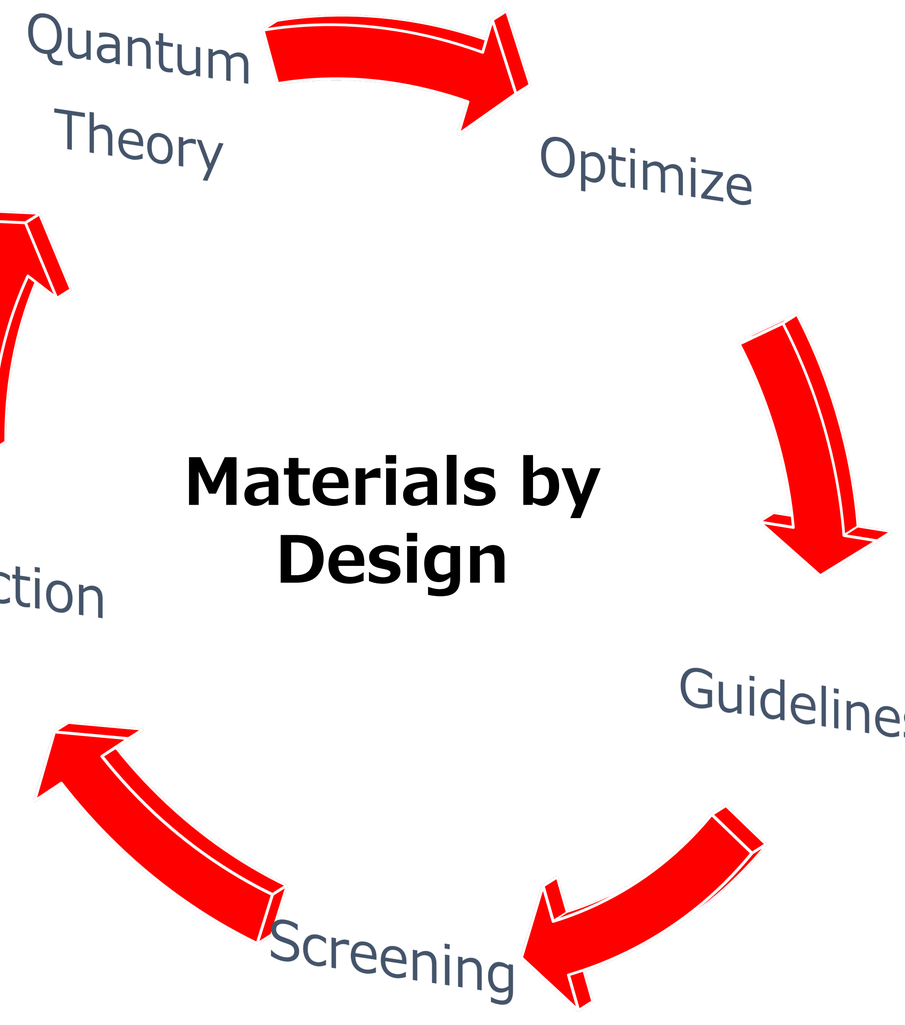
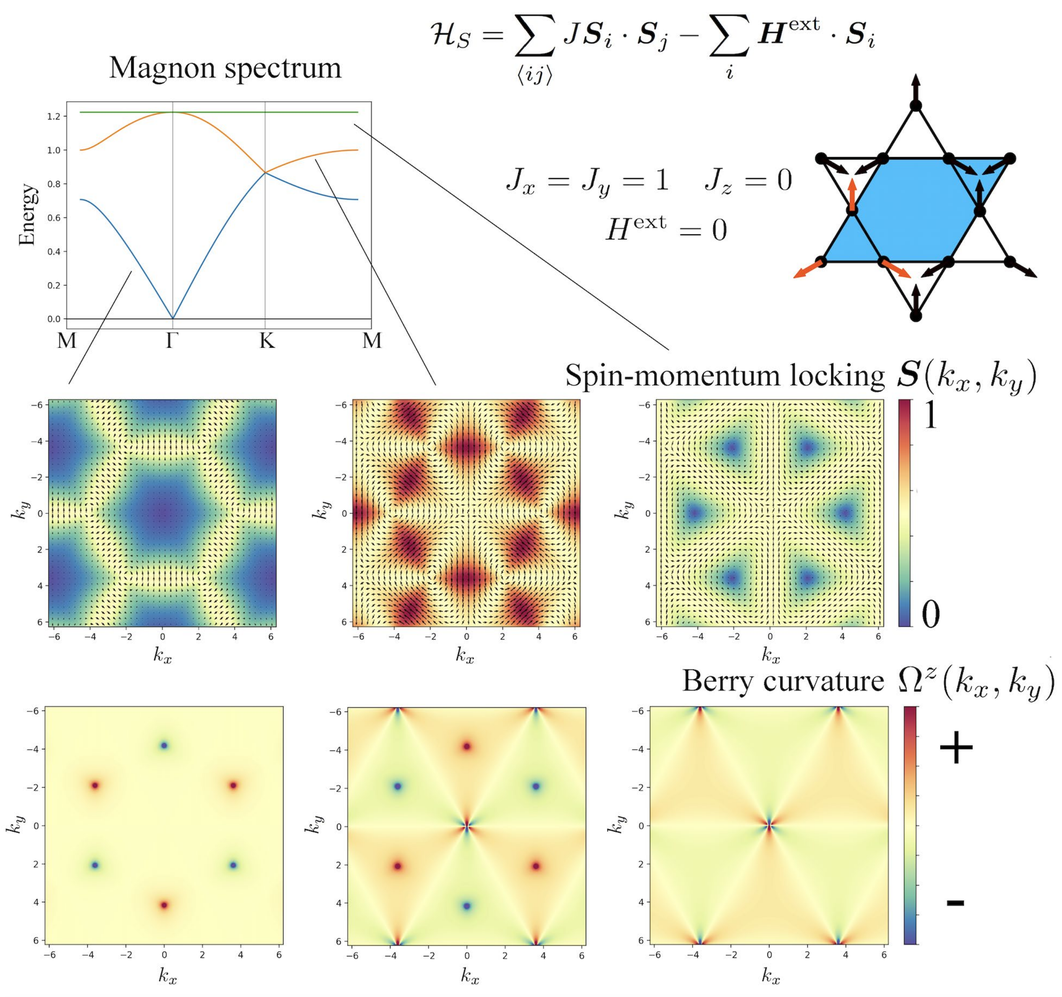
- Magnetic and magnetoelectric phenomena
- Investigation of spin dependent phenomena
- Atomic order/disorder vs. Properties of materials
- Novel meta-stable phases

Unravel the material-property duality based on materials specific quantum mechanical calculations, this being, the fundamental step in the designing of new materials with new and/or enhanced magnetic functionalities.

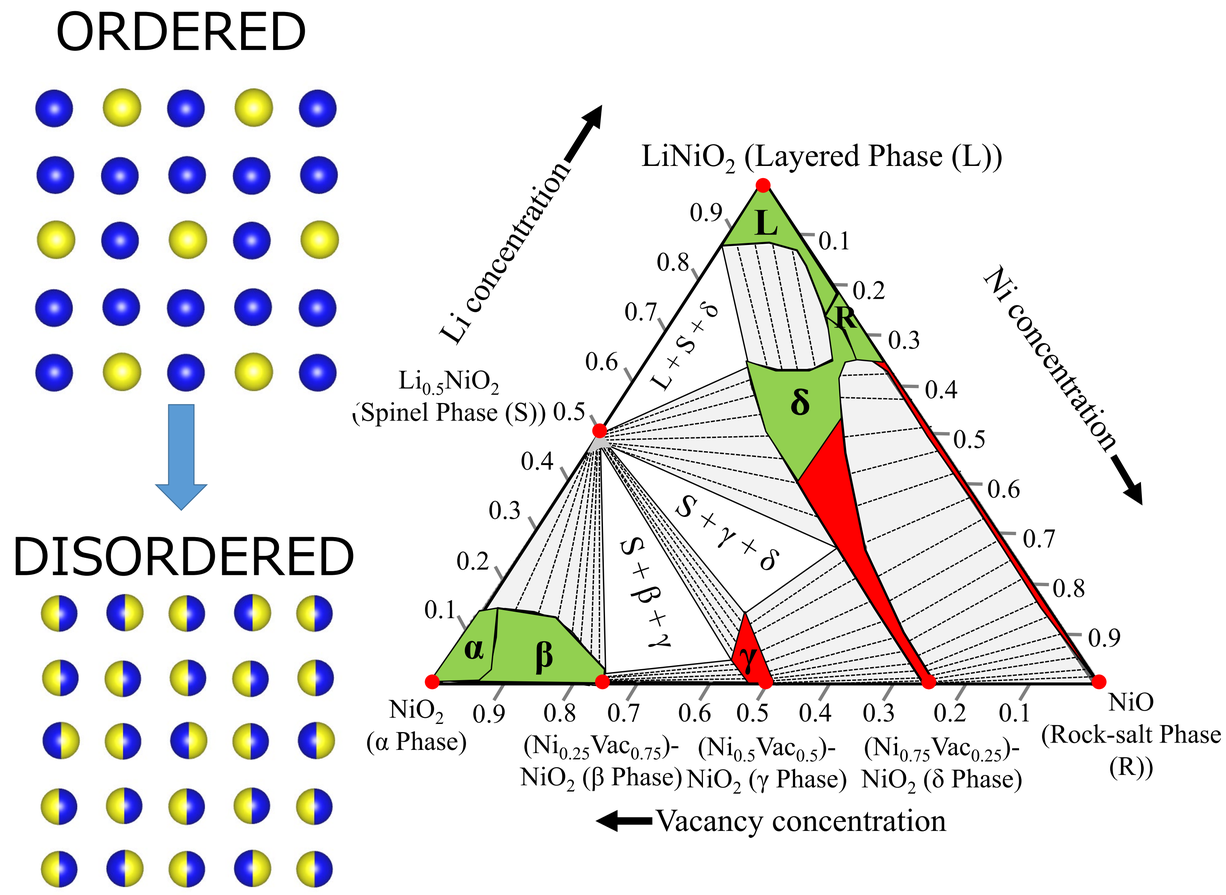
∘ Magnetic phenomena, ∘ Magnetoelectric phenomena, ∘ Topological phases, ∘ Spin dependent phenomena, ∘ Ionic transport, ∘ Negative thermal expansion





We construct materials specific models to study various quantum phenomena in materials : Thermal Hall effect, Spin Seebeck effect, Spin Nernst effect

Nature Communications **5**, 2998 (2014);
Nature Materials **13**, 163-167 (2014),
Nature **537**, 523–527 (2016)



We study thermodynamic and kinetic phase stability of ordered/disordered phases and their control over the properties of materials

Chem. Mater. **29**, 7840-7851 (2017),
Chem. Mater. **31**, 4748-4758 (2019)