

Hybrid perovskite: Structural prototypes and DFT

Hybrid perovskites have attracted considerable interest recently for their exceptional optoelectronic properties and potential applications in photovoltaics, light-emitting devices, and photodetectors, making them highly promising for next-generation technologies. In this project, AiiDA workflow manager and VASP will be used to conduct high-throughput calculations to identify stable and high-performance two-dimensional (2D) perovskites.

This research focuses on the generation of 2D perovskite structures across different structural prototypes, including Ruddlesden-Popper (RP) and Dion-Jacobson (DJ) phases. The primary objective of this project is to investigate physical properties, such as shift current [1], in screened perovskite candidates. Consequently, this project necessitates a strong motivation to work with various tools, including AiiDA [5], VASP [3, 2], Wannier90 [4], and Python.

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References

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