



Contribution ID: 147

Type: **Talk**

【108】 Tuning the Electronic Properties of Two-Dimensional Lepidocrocite Titanium Dioxide-Based Heterojunctions

Tuesday 10 September 2024 15:45 (15 minutes)

This study investigates a 2D Janus heterostructure made by combining lepidocrocite TiO₂ and MoSSe, focusing on the energetic stability and change in electronic properties with respect to varied interface terminations. Using state-of-the-art density functional theory simulations, we show that TiO₂-MoSSe heterostructures are energetically feasible to form. The results indicate that by varying the atomic species at the interface, the electronic structure can be considerably altered due to the differences in charge transfer arising from the inherent electronegativity of the atoms. The work demonstrates that the Janus interface enables the tuning of electronic properties, providing an understanding of the possible applications of the TiO₂-MoSSe heterostructure.

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Session Classification: Condensed Matter Physics (KOND)

Track Classification: Condensed Matter Physics (KOND)