

## The MGI First Principles Phase Stability Repository; and recent studies of exotic order-disorder transitions.



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**NIMS 並木地区**

**WPI-MANA棟 Auditorium**

The First Principles Phase Stability Repository

<http://nist.matdl.org/dspace/xmlui/> was created to enhance reproducibility and reuse of calculations in which many (tens, hundreds, etc.) electronic structure calculations (typically DFT) are used to fit effective Hamiltonians, with which one can model finite-T properties (e.g. first principles phase diagram calculations; fitting empirical- or tight-binding-potentials to FP calculations).

Essentially, the idea is to upgrade publications of such studies to the point that reproduction or reuse requires only hours or days rather than months. Two examples of exotic order-disorder phenomena will also be discussed: 1) interstitial order-disorder of oxygen and vacancies in hexagonal Ti, Zr and Hf; 2) the prediction of aperiodic (incommensurate) phases in the 2D system  $\text{MoS}_2\text{-MoTe}_2$ .

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