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Contrasting structural and electrical phase transition behaviors of layered transition metal dichalcogenides $MoTe_2$ and WTe_2

Layered transition metal dichalcogenides $MoTe_2$ and WTe_2 share almost similar lattice constants as well as topological electronic properties except their structural phase transitions. While the former shows a first-order phase transition between monoclinic and orthorhombic structures, the latter does not. Using a recently proposed van der Waals density functional method [1], we investigate structural stability of the two materials and uncover that the disparate phase transitions originate from delicate differences between their interlayer bonding states near the Fermi energy [2]. By exploiting the relation between the structural phase transitions and the low energy electronic properties, we show that a charge doping can control the transition substantially, thereby suggesting a way to stabilize or to eliminate their topological electronic energy bands.

References

1. I. Hamada, Phys. Rev. B, 89 (2014) 121103.
2. H.-J. Kim, S.-H. Kang, I. Hamada, and Y.-W. Son, Phys. Rev. B, 95 (2017) 180101(R).

Figures

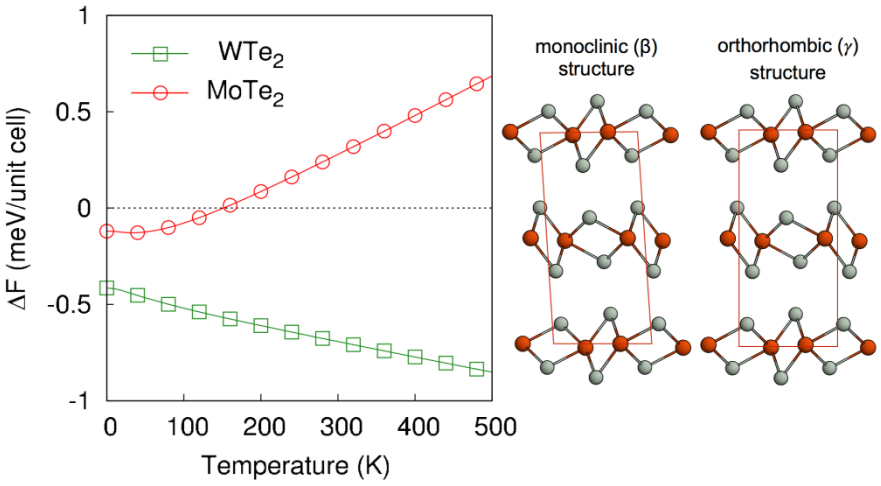

Figure 1: Calculated free energy difference $\Delta F = F_\gamma - F_\beta$ between monoclinic (β) and orthorhombic(γ) structure, where $F_{\beta(\gamma)}$ is a free energy of β(γ) structure.