Multiferroic Orders in Two-dimensional Materials

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Abstract

In this talk, we present that the twodimensional tin monoxide (a-SnO) have valence band with a Mexican-hat shape and van Hove singularities (vHS) diverging with $1/\sqrt{E}$ [1], as shown in **Fig. 1**. The vHS observed at the top of valence band create an electronic instability that cause some phase transitions.

We show that changing the hole doping, the a-SnO monolayer can be ferroelastic and/or ferromagnetic. And that through a effective simple model, the energy difference between the ferromagnetic and non-magnetic states calculated are similar to those calculated by first principles methods. Thus, these results can be extended to other 2D materials with valence band with Mexican-hat shape, as GaS [2] and GaSe [3].

Also, we show that the phase transitions observed in a-SnO can be described by a generalized Landau model, as shown in Fig. 1(c).

Finally, we show that acceptor point defects can also induce phase transitions in **a**-SnO depending on the number of layers, and defect concentrations.

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References

- L. Seixas, A. S. Rodin, A. Carvalho, A. H. Castro Neto, *Phys. Rev. Lett.* **116**, 206803 (2016).
- [2] S. Wu et al., arXiv:1409.4733
- [3] T. Cao, Z. Li, and S. G. Louie, *Phys. Rev. Lett.* **114**, 236602 (2015).



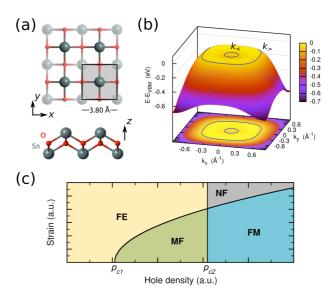


Figure 1: (a) Schematic representation of a-SnO monolayer from top view (top panel) and side view (bottom panel). (b) Mexican-hat valence band surface of a-SnO monolayer. (c) Phase diagram based on generalized Landau model for multiferroicity in a-SnO monolayer.