Multiferroic Orders in Two-dimensional Materials

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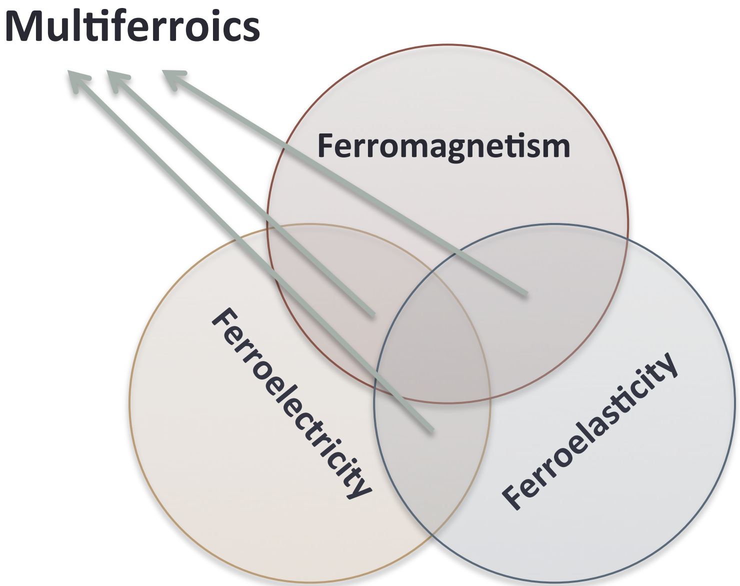
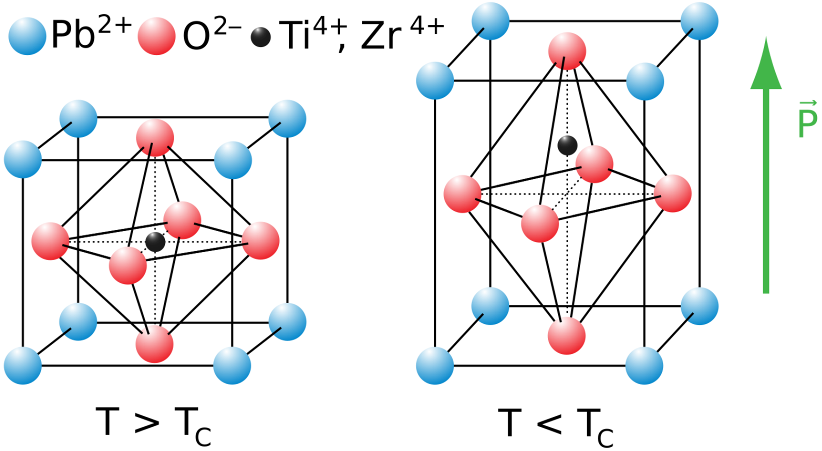
Multiferroics





Perovskite

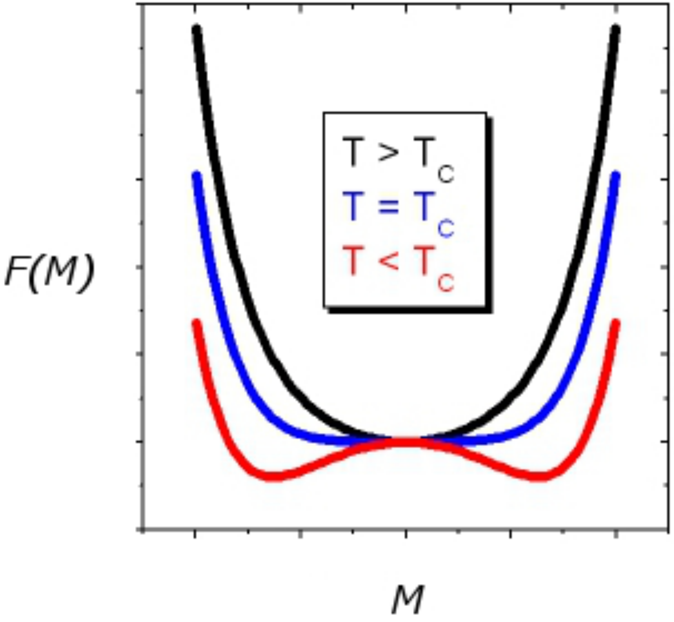
Landau theory

$$F(\mathcal{M}) = \alpha(T)\mathcal{M}^2 + \beta\mathcal{M}^4$$

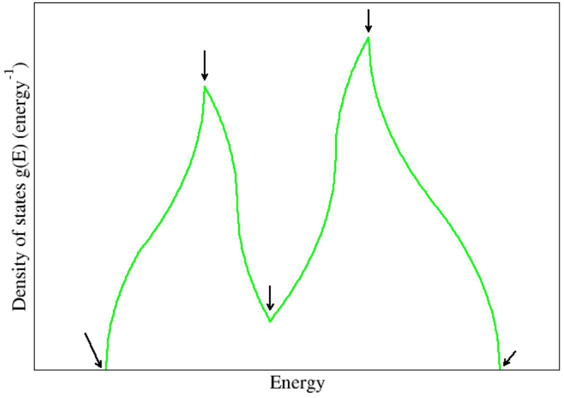
$$\frac{\partial F}{\partial \mathcal{M}} = 0 \Rightarrow \alpha(T)\mathcal{M} + 2\beta\mathcal{M}^3 = 0$$

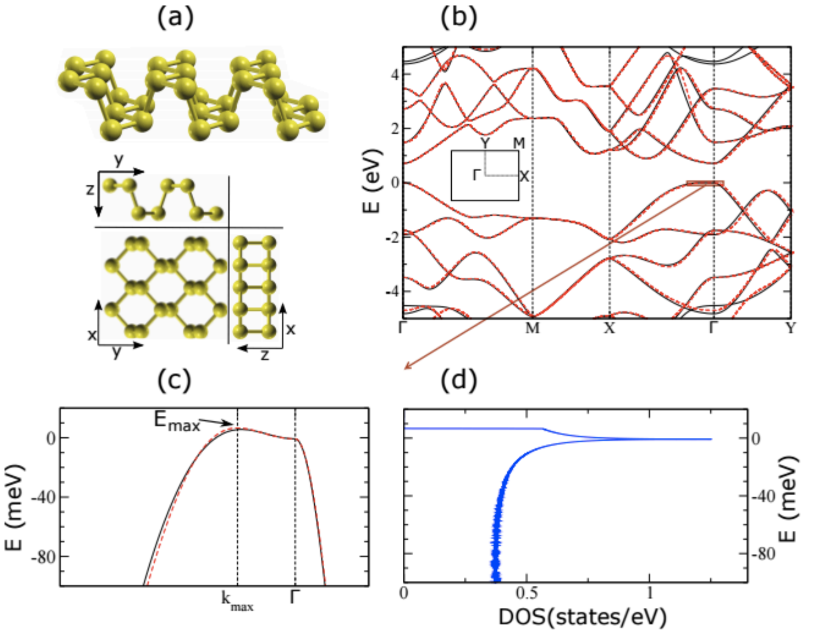
$$\mathcal{M} = 0, \;\; \mathcal{M} = \pm\sqrt{-\frac{\alpha(T)}{2\beta}}$$

$$\alpha(T) = \alpha_0(T - T_C)$$



van Hove singularities (VHS)





A. Ziletti *et al*. Phys. Rev. B **92**, 085423 (2015)

Stoner criterion

$$DOS(E_F)U > 1$$

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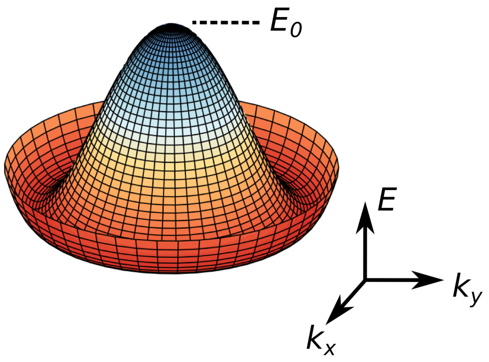
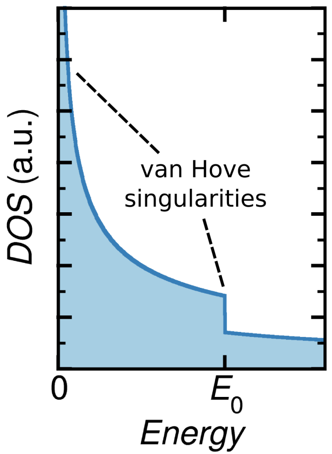
Mexican-hat band edge (MHBE)





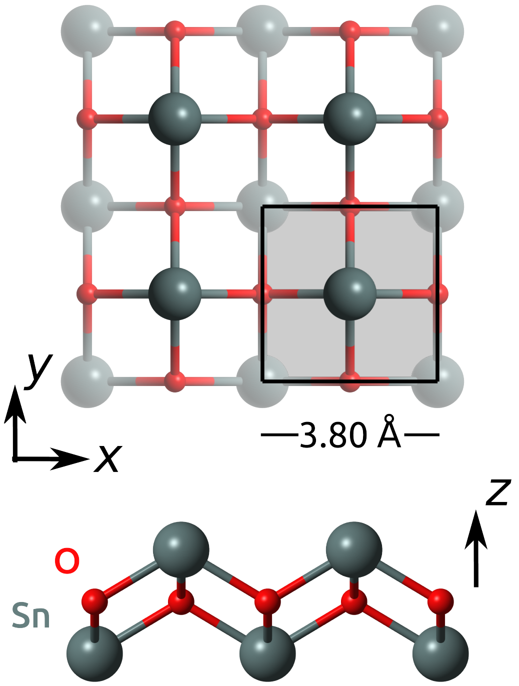
Band edge

$$E(k) = Ak^4 + Bk^2 + E_0,$$

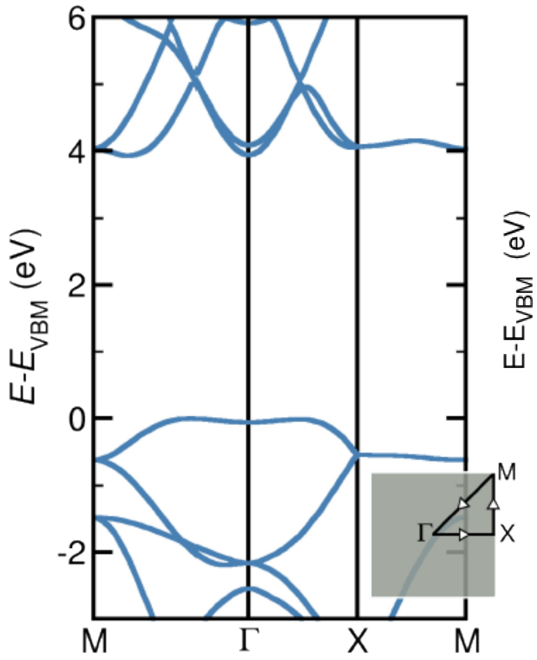
Density of states

$$DOS(E) = \frac{1}{4\pi\sqrt{A}}\frac{1}{\sqrt{E}}\left[1 - \frac{\Theta(E - E_0)}{2}\right]$$

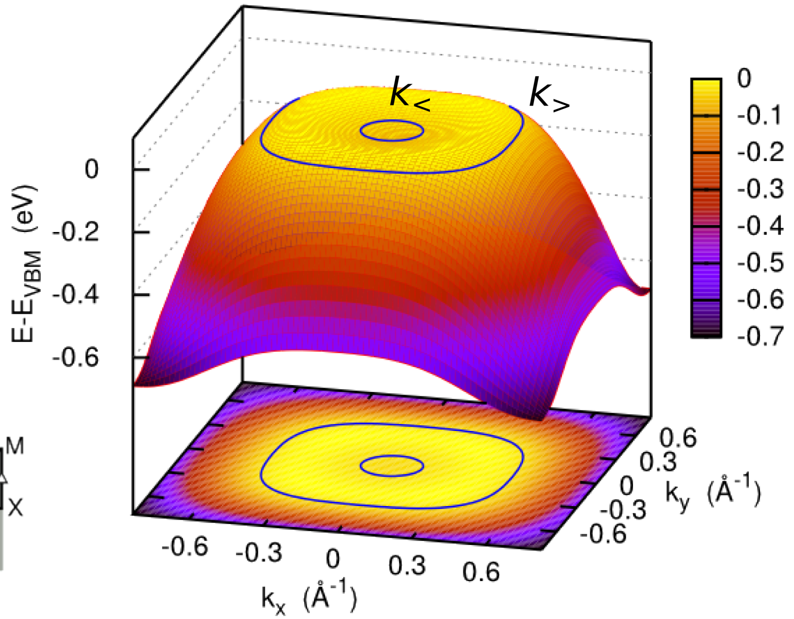
α-SnO



y
x
—3.80 Å—
z
O
Sn

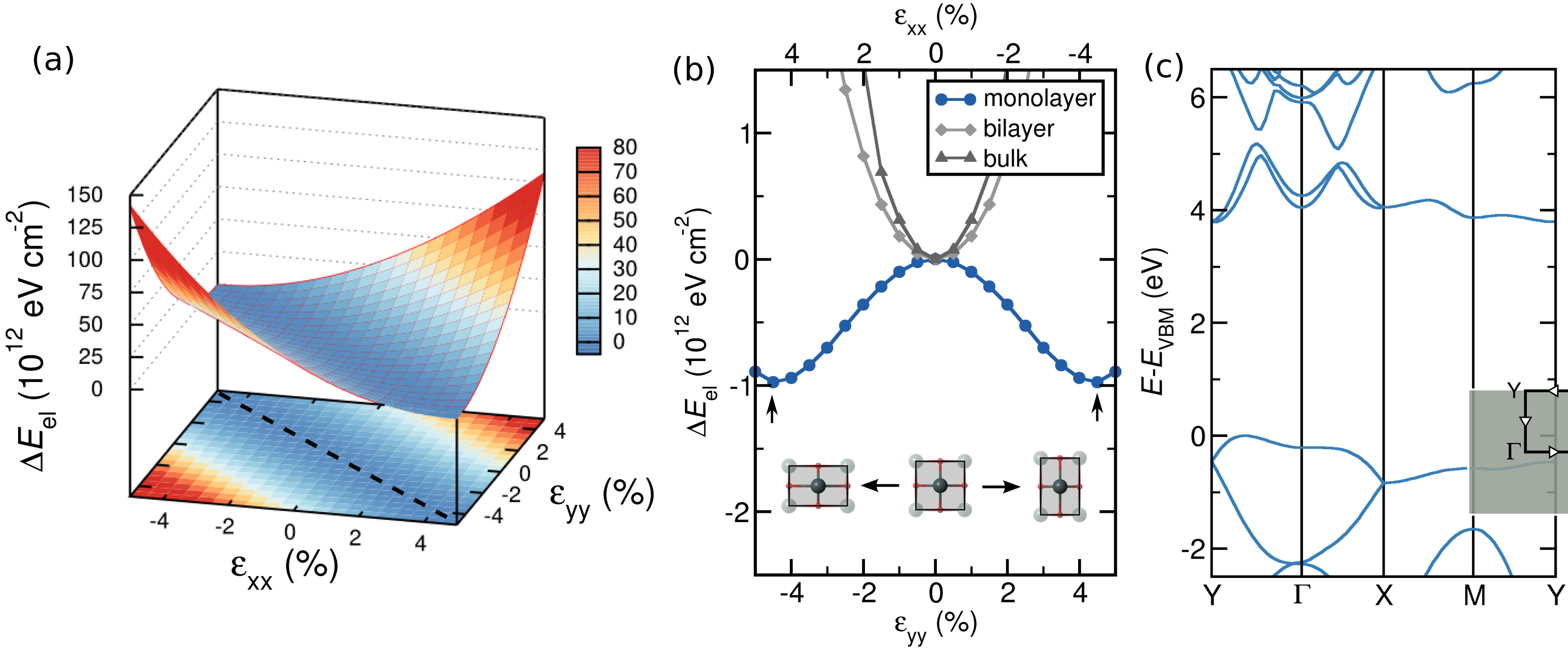


6
4
2
0
-2
E-E_VBM (eV)
M
Γ
X
M



k<
k>
0
-0.2
-0.4
-0.6
E-E_VBM (eV)
0
-0.1
-0.2
-0.3
-0.4
-0.5
-0.6
-0.7
-0.6
-0.3
0
0.3
0.6
k_x (Å^-1)
0.6
0.3
0
-0.3
-0.6
k_y (Å^-1)

Ferroelasticity in α-SnO



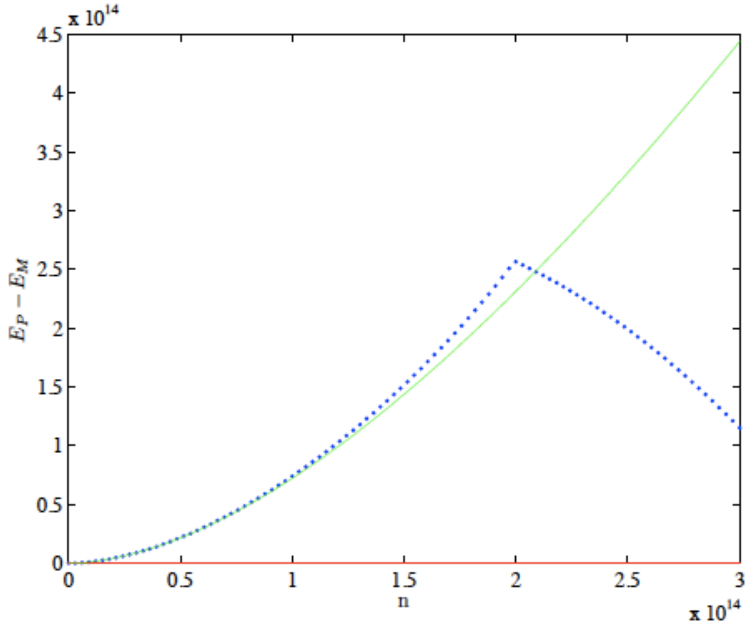
Ferromagnetism (Analytical model)

Magnetic system

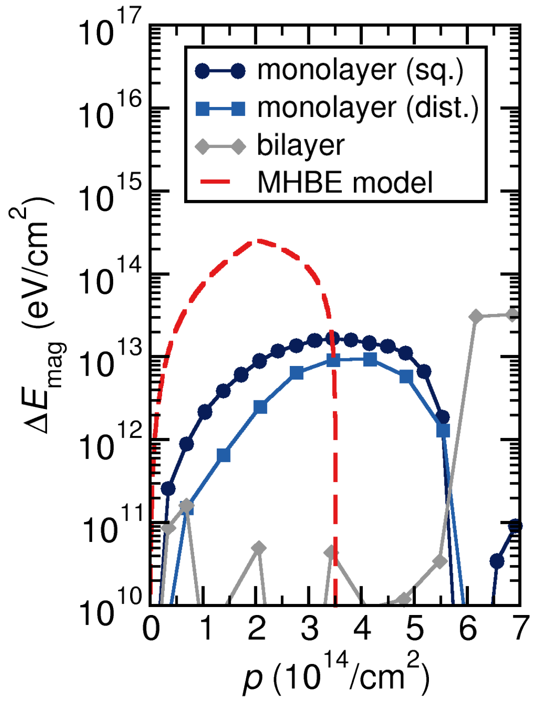
$$\mathcal{E}^{\mathrm{M}}_{\mathrm{system}}(n) \approx n^2 \left\{ \frac{4\pi^2 A}{3} n - e^2 \left(3 + 2 \ln \left(\frac{2B}{An\pi} \right) \right) \sqrt{\frac{A}{2B}} \right\}$$

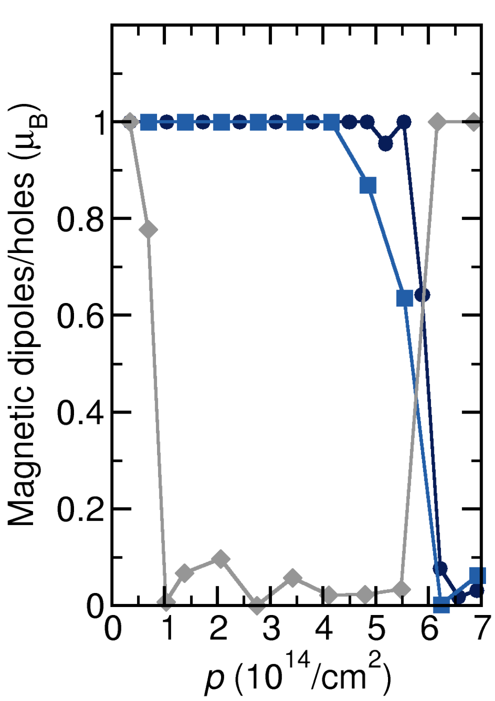
Non-magnetic system

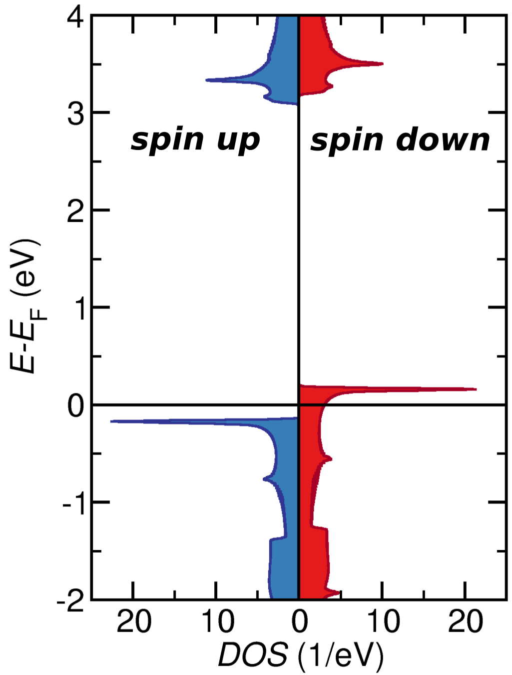
$$\mathcal{E}^{\mathrm{U}}_{\mathrm{system}}(n) \approx 2 \left[\left(\frac{n}{2} \right)^2 \left\{ \frac{2\pi^2 A}{3} n - e^2 \left(3 + 2 \ln \left(\frac{4B}{An\pi} \right) \right) \sqrt{\frac{A}{2B}} \right\} \right]$$



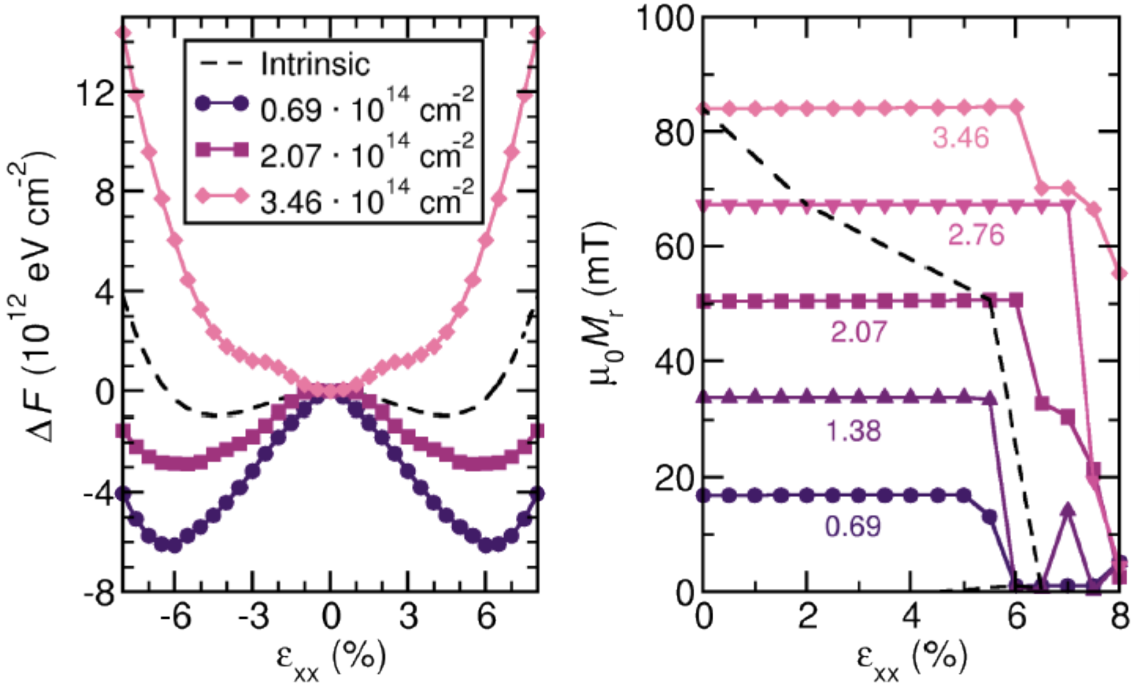
Ferromagnetism in α-SnO







Multiferroicity in α-SnO



Ferroelasticity
+
Ferromagnetism

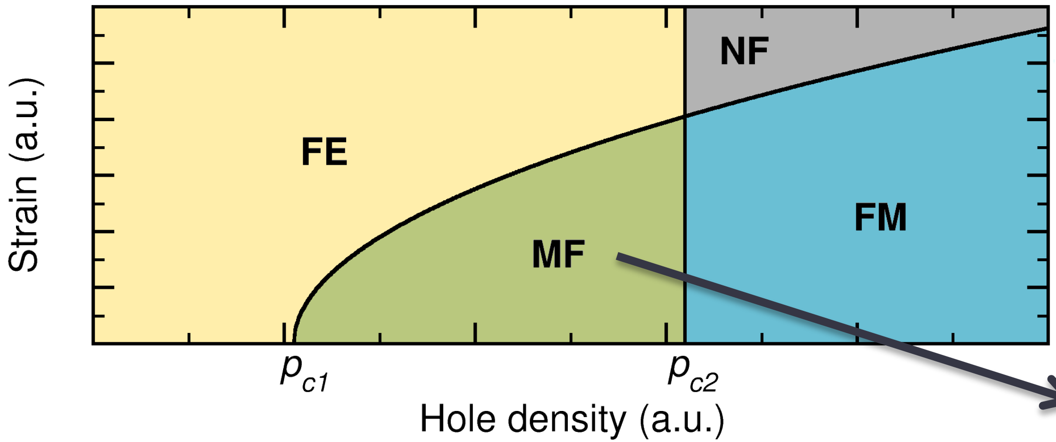
Landau theory of α-SnO

Ferromagnetic **Ferroelastic**

$$F(\mathcal{M},\varepsilon) = \alpha(p)\mathcal{M}^2 + \beta\mathcal{M}^4 + \gamma\varepsilon^2\mathcal{M}^2 + \eta(p)\varepsilon^2 + \lambda\varepsilon^4$$

$$\alpha(p) = \alpha_0\,(p_{c1} - p)$$

$$\eta(p) = \eta_0\,(p - p_{c2})$$



$$\varepsilon_{pt} = \sqrt{\frac{\alpha_0}{\gamma}(p - p_{c1})}$$

Multiferroicity

Summary

- 2D materials with Mexican-hat band edge can became ferromagnetic with free carrier densities;
- α-SnO is ferroelastic for monolayer;
- α-SnO can be multiferroic for *p*-type doped material.
- **α-SnO monolayer is the first 2D material multiferroic with ferromagnetism and ferroelasticity.**

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FAPESP

Thank you!