In 2D: Ferroelectric Switch of Electronic Topology, and the Flexo-Ferroelectricity of Actuator Motor

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The low dimensionality (of 1D nanowires [1] or 2D monolayers [2-4]) brings about two distinctly new features to ferroelectric: (I) its polarization ***P*** can be along, longitudinal (***P***$_l$) or perpendicular, transverse (***P***$_t$) with respect to the material line or plane—a strong anisotropy due to low-D, absent for 3D crystals. (II) Compliance, to bend easily into "empty-dimension", a new degree of freedom on display. We discuss examples, emerging from (I) and (II), where flipping intrinsic ***P*** switches something else—the essence of multiferroics, where electrical and magnetic polarizations are coupled (also possible in low-D, e.g. in MXene [2]). We show how ±***P***$_t$ flip switches the topological state of 2DM [3] or, in very different manifestation, can alter the shape, performing as actuator [4].

We design and explore with DFT a hetero-bilayer of realistic 2D components of matching lattice symmetry, the β-phase antimonene β-Sb (known for its strong spin−orbit coupling) and ferroelectric In_2Se_3. The ±***P*** of the In_2Se_3 induces distinctly different electronics in the bilayer: if ***P*** points "inward", the bilayer is a trivial insulator; when switched "outward", its state is nontrivial topological, $Z_2 = 1$ — inviting future multifunctional devices' applications [3].

In another striking example, the often-overlooked (blocked by the substrate) flexibility of 2DM leads to unexpected behavior of the ferroelectrics. We introduce a "ferro-flexo" coupling term $\sim P\cdot\kappa$ into the Ginzburg-Landau-Devonshire φ^4-energy, to connect the ferroelectricity and curvature, κ. The DFT and Monte-Carlo methods allow one to quantify all parameters, so to predict the spontaneous curvature κ_s and the effects on phase transition (rising Curie temperature, domain wall width, etc.) for InP, $CuInP_2S_6$ and In_2Se_3 as chemically-specific representatives. Polarization switches do bend the layer, converting electrical signal to movement as an actuator, with efficient work-cycle.

References

[1] J.-J. Zhang, et al., B.I.Y., J. Am. Chem. Soc., 141 (2019) 15040
[2] J.-J. Zhang, et al., B.I.Y., J. Am. Chem. Soc. 140 (2018) 9768
[3] J.-J. Zhang, et al., B.I.Y., Nano Lett. 21 (2021) 785
[4] J.-J. Zhang, et al., B.I.Y., ACS Nano, (2023) doi.org/10.1021/acsnano.3c00492

Figures

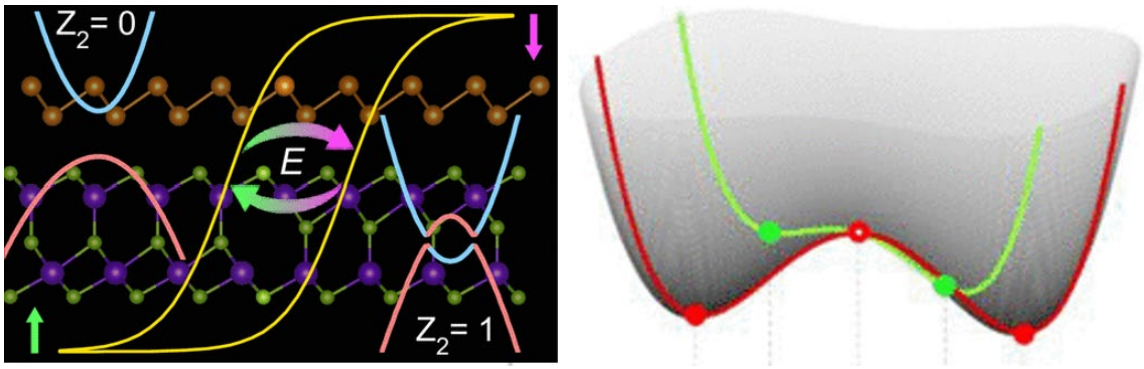

Figure 1: Left: The hysteresis of *P*, switching the topological state [3]. Right: The generalized φ^4-potential surface $U(P,\kappa)$ of a 2DM flexo-ferroelectric, flat (green) or with relaxation (red) [4].