Constructive coupling effect of topological states and topological phase transitions in plumbene

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Abstract

Combining tight-binding (TB) models with first-principles calculations, we investigate electronic and topological properties of plumbene. "Constructive" coupling effects of topological states are found in the low-buckled plumbene, causing the system being a normal insulator, opposite to topologically nontrivial states formed in other two-dimensional (2D) group IVA monolayers (from graphene to stanene). Local topologic states are found being located not only at the Γ point in the Brillouin zone, but also at the *K/K'* points, whose coupling determines the final topological behaviors of the whole system. Based on this mechanism, several schemes are raised to produce a globally topological state in the plumbene. When the plumbene is functionalized with ethynyl (PbC_2H), a quantum spin Hall (QSH) state comes out. Very interestingly, when an exchange field is introduced to the pristine plumbene, the system exhibits a quantum anomalous Hall (QAH) effect despite the coupling effect of the topological states.

Geometry structures

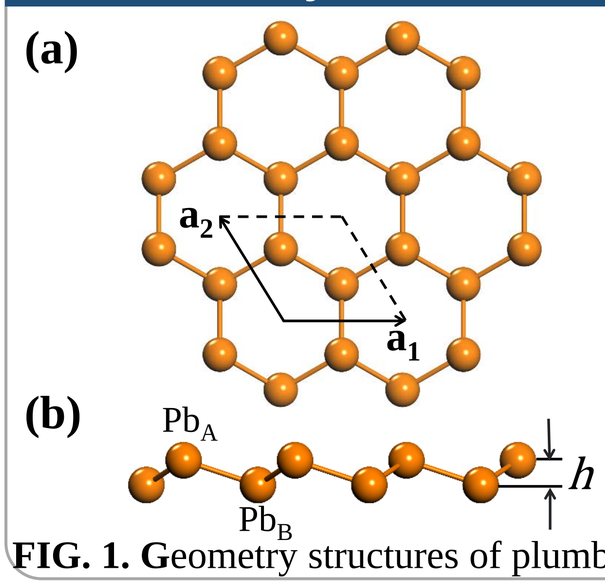


FIG. 1. Geometry structures of plumbene.

Band structures and edge states

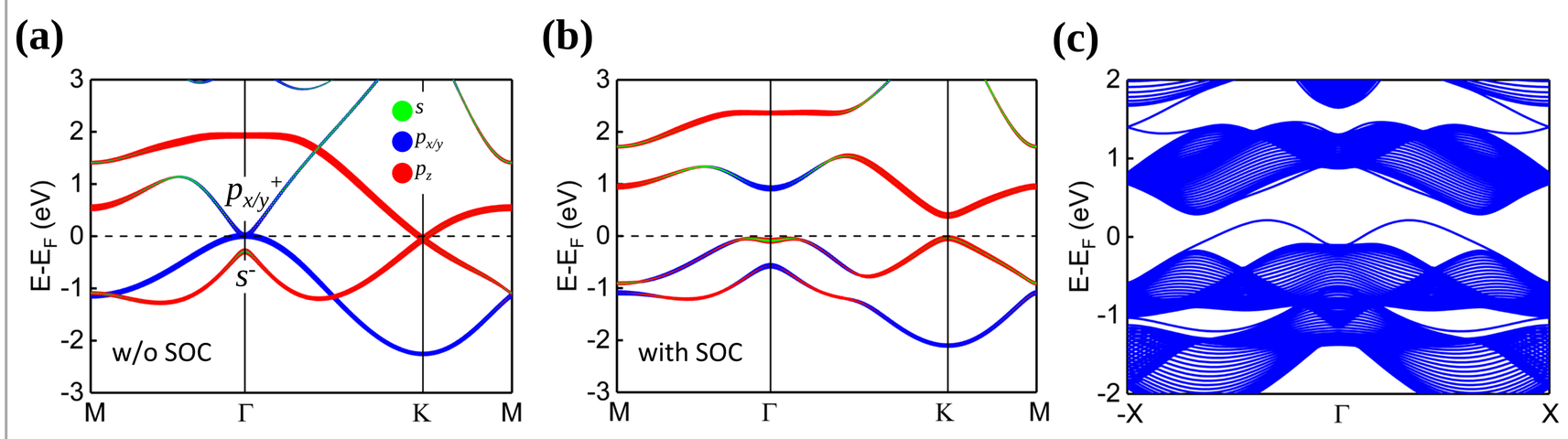


FIG. 2. (a) and (b) Orbital-projected band structures, and (c) edge states of plumbene.

Coupling effect of topological states from tight-binding model

Tight-binding model

$$H(\boldsymbol{k}) = \sum_{<ij>,\alpha,\beta;\sigma,\sigma'} c^{\dagger}_{\alpha\sigma i} t_{\alpha\sigma i;\beta,\sigma' j}\, c_{\beta\sigma' j} + \lambda \mathrm{L}\cdot\mathrm{S} + M \sum_{i;\alpha;\sigma,\sigma'} c^{\dagger}_{\alpha\sigma i} s^{z}_{\sigma\sigma'} c_{\alpha\sigma' i}$$

Topological properties

$$\Omega_{\alpha\beta}(\boldsymbol{k}) = \sum_n f_n \Omega_{n,\alpha\beta}(\boldsymbol{k})$$

$$\Omega_{n,\alpha\beta}(\boldsymbol{k}) = -2\mathrm{Im}\sum_{m\neq n} \frac{\hbar^2 \langle\psi_{n\boldsymbol{k}}|v_\alpha|\psi_{m\boldsymbol{k}}\rangle\langle\psi_{m\boldsymbol{k}}|v_\beta|\psi_{n\boldsymbol{k}}\rangle}{\left(\mathrm{E}_m(\boldsymbol{k})-\mathrm{E}_n(\boldsymbol{k})\right)^2}$$

$$C = \frac{1}{2\pi}\sum_n \int_{BZ} d^2k \Omega_n$$

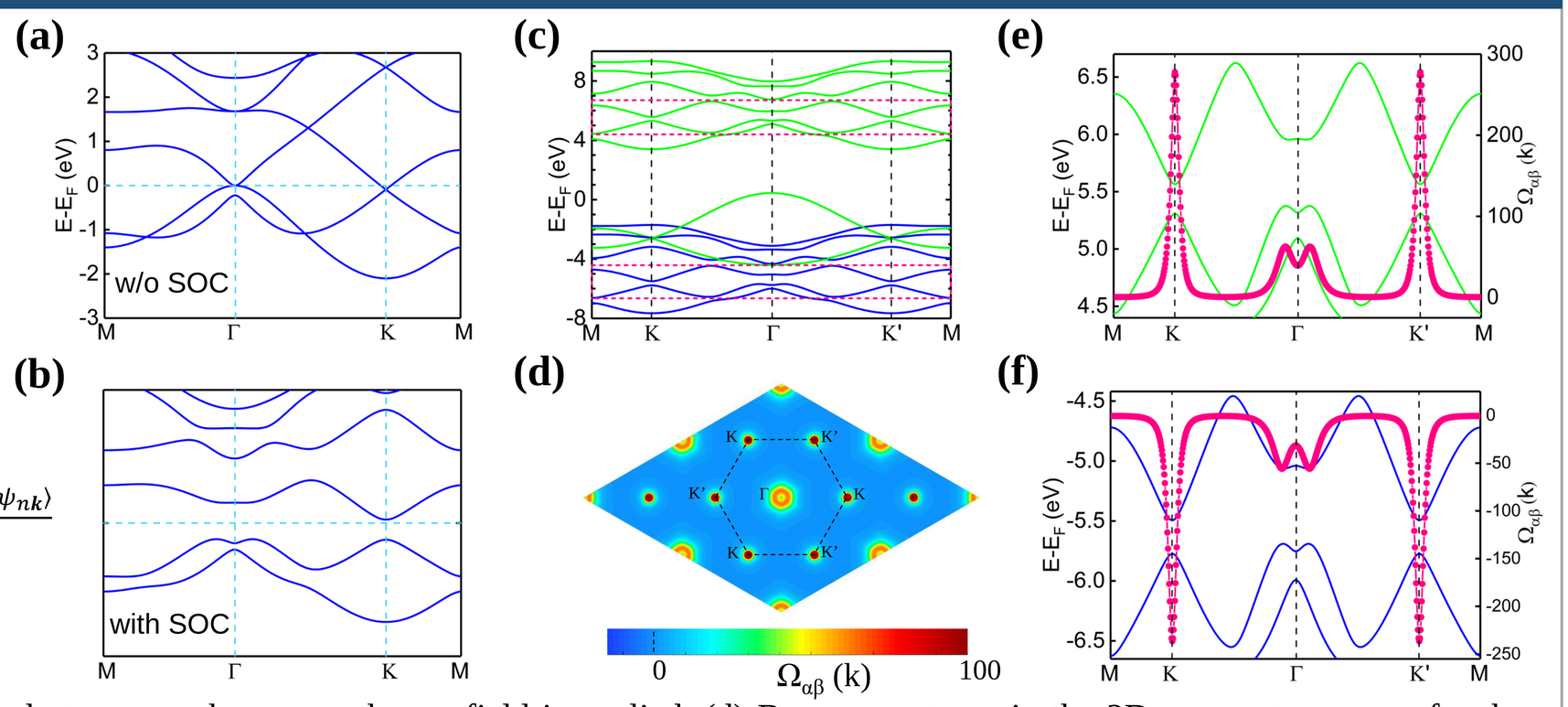
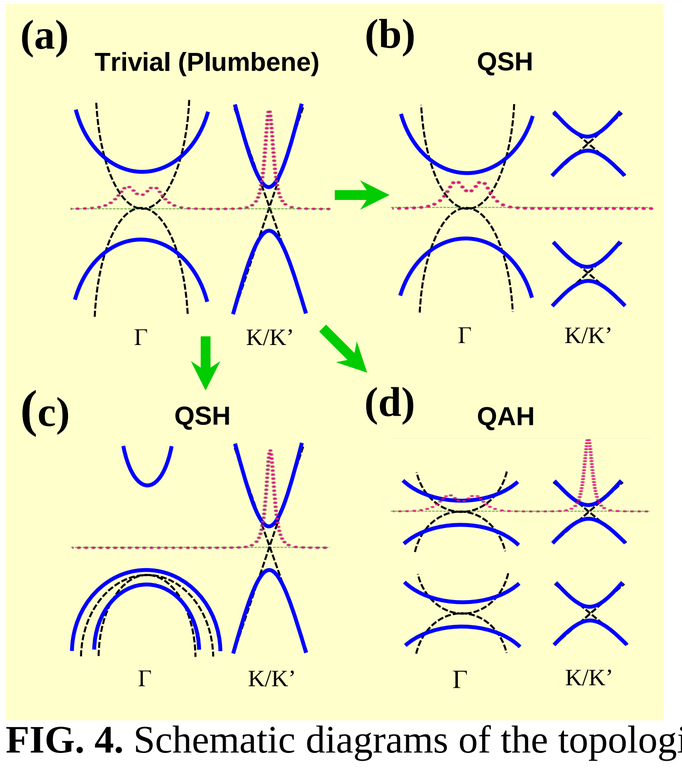


FIG. 3. (a) and (b) Band structures, (c) band structure when an exchange field is applied, (d) Berry curvatures in the 2D momentum space for the spin-up subspace, (e) and (f) Berry curvatures and bands for the spin-up and spin-down subspace, respectively, obtained from TB model.

Topological phase transitions



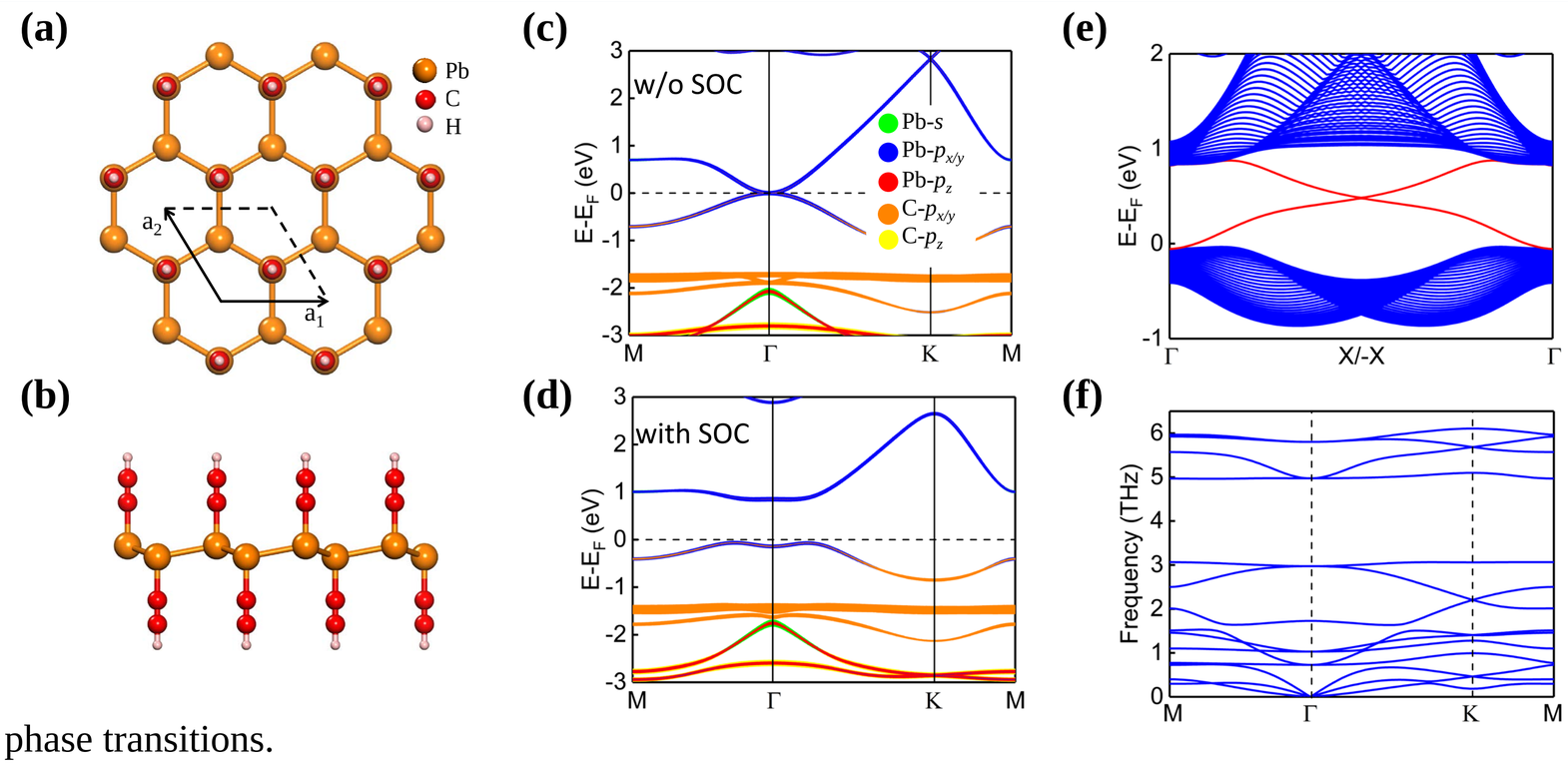


FIG. 4. Schematic diagrams of the topological phase transitions.

FIG. 5. (a) and (b) Geometry structures, (c) and (d) orbital-projected band structures, (e) edge states, and (f) phonon band dispersions of PbC_2H.

References:

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