Supplementary materials for Coexistence of Triple Nodal Points, Nodal Links, and Unusual Flat Band in intermetallic $\mathcal{A}\mathrm{Pd}_3$ ($\mathcal{A}$=Pb, Sn)

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Additional details that were mentioned in the main text are provided here, with description in the figure captions.

FIG. 1: Blowup plots corresponding to Figs. 2a and 2b in the main text.

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FIG. 2: Band structures, corresponding to Figs. 2a and 2b, along the $X - \Gamma - M - X$ line.
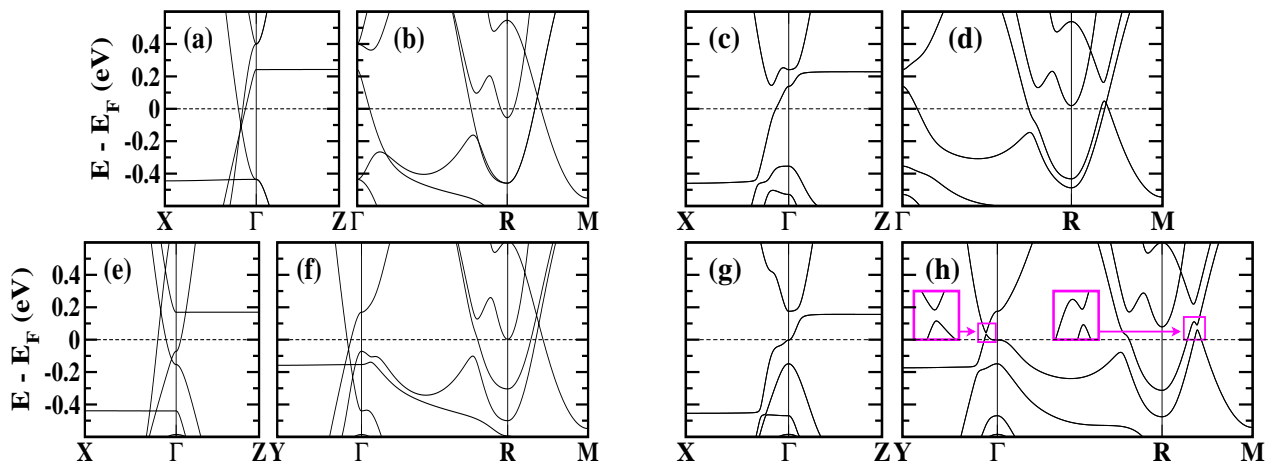

FIG. 3: Enlarged band structures of PbPd$_3$ for tetragonally (top) and orthorhombically (bottom) distorted structures. The panels of (a), (b), (e), and (f) are in GGA, while the panels of (c), (d), (g), and (h) in GGA+SOC. For comparison, the notation of the high symmetry points follows that of the cubic case. The X, Y, and Z points are the zone boundary of (100), (010), and (001), respectively. For the tetragonal case, the C_{3v} symmetry is broken along (111) direction. In the orthorhombic case, the C_{4v} symmtery is also broken along (110) direction at $k_z = \pi/c$ plane. Although anticrossings at TNPs occur evern for a small distortion, for a better visualization these figures are given for large distortions: the ratio of lattice parameters of 1:1.1 for the thetraonal structure and of 1:1.05:1.1 for the orthrombic structure.
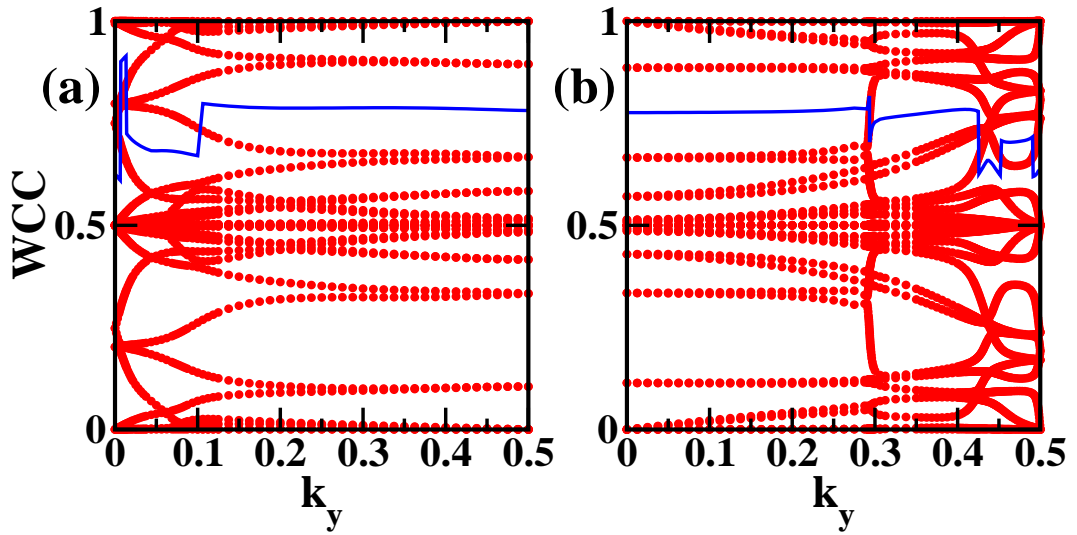
FIG. 4: For the tetragonally distorted structure, plot of the hybrid Wannier charge centers (HWCCs) plot (red, thick lines) across half of the Brillouin zone in the (a) $k_z = 0$ and (b) π/c plane, showing an even number of crossings between the charge center and largest gap (blue, thin line) among two adjacent HWCCs. The orthorhombic case shows similar behavior, so the figure is not repeated here. The magnitude of the wave vector k_y in the horizontal axis is given in the unit of π/a.
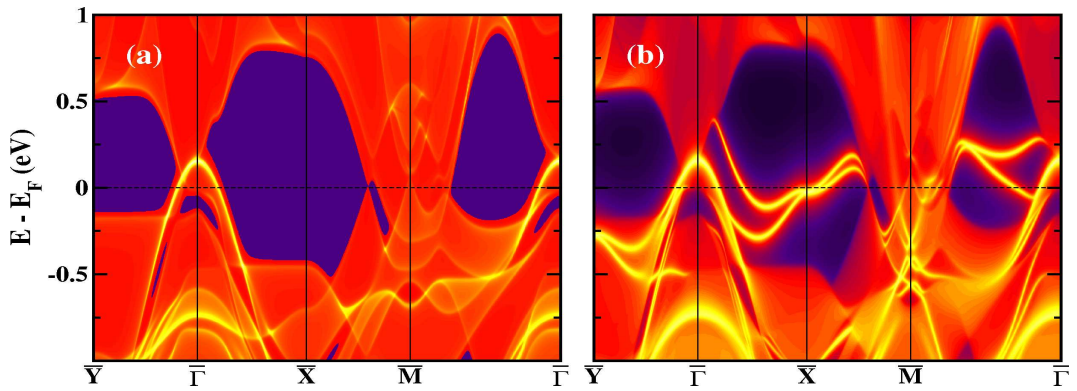

FIG. 5: The bulk-only contribution (left) to the (001) surface spectral function (right) for Pd_2 termination of the orthorhombic case in GGA+SOC. Compared with two plots, two surface states appear in-gap, indicating a topological nontrivial state.
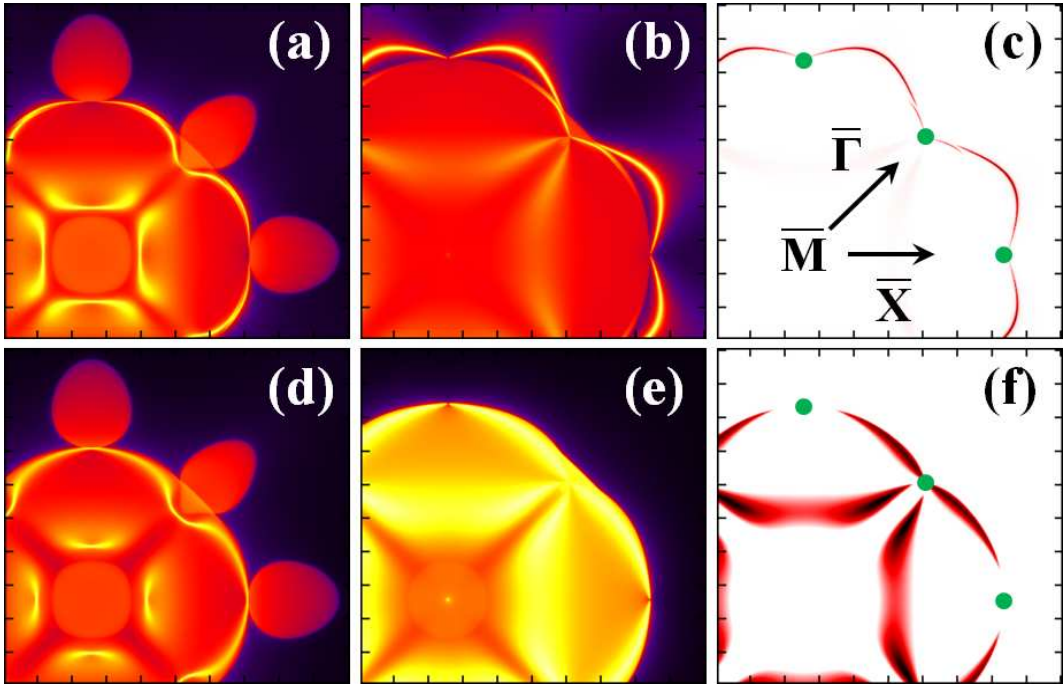
FIG. 6: Enlarged $\bar{M}$-centered (001) surface spectral functions for (top) Pd$_2$ and (bottom) Pb-Pd terminations in GGA. The strong yellowish lines denote surface states. Panels (a) and (d) indicate states at the Fermi energy E_F; (b) and (e) indicate states at 0.18 eV where the triple nodal points (TNPs) appear. Panels (c) and (f) selects only the surface contribution of (b) and (e) respectively. The R-centered spheroid is connected to four protrusions by Fermi arcs. In panels (c) and (f), the green dots denote TNPs.
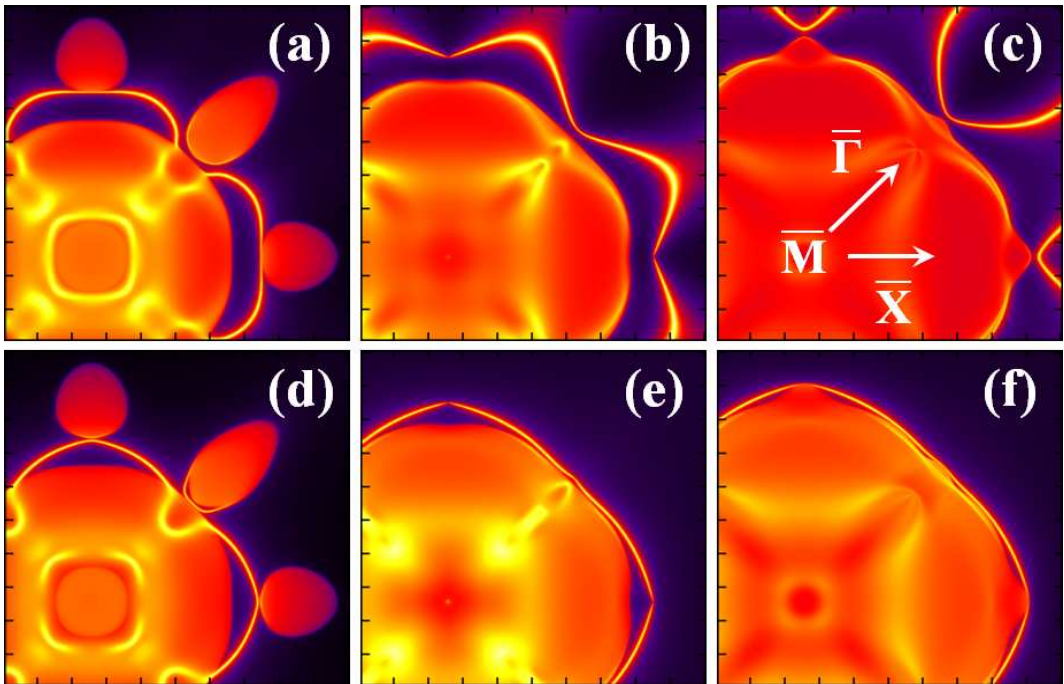

FIG. 7: Enlarged $\bar{M}$-centered (001) surface spectral functions for (top) Pd$_2$ and (bottom) Pb-Pd terminations in GGA+SOC. Panels (a) and (d) are at E_F. Panels (b) and (e) are at 0.14 eV, crossing the Dirac point along the $R - M$ line. Panels (c) and (f) are at 0.22 eV, crossing the Dirac point along the $\Gamma - R$ line.