Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

— Supplementary Information —

Tuning Valley Degeneracy in Rock-Salt IV-VI Compounds with Band Inversion

Michael Y. Toriyama,*,† Madison K. Brod,† Lídia C. Gomes,‡ Ferdaushi Alam Bipasha,‡ Badih A. Assaf,¶ Elif Ertekin,‡ and G. Jeffrey Snyder†

†*Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208*

‡*Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801*

¶*Department of Physics, University of Notre Dame, Notre Dame, IN 46556*

E-mail: MichaelToriyama2024@u.northwestern.edu

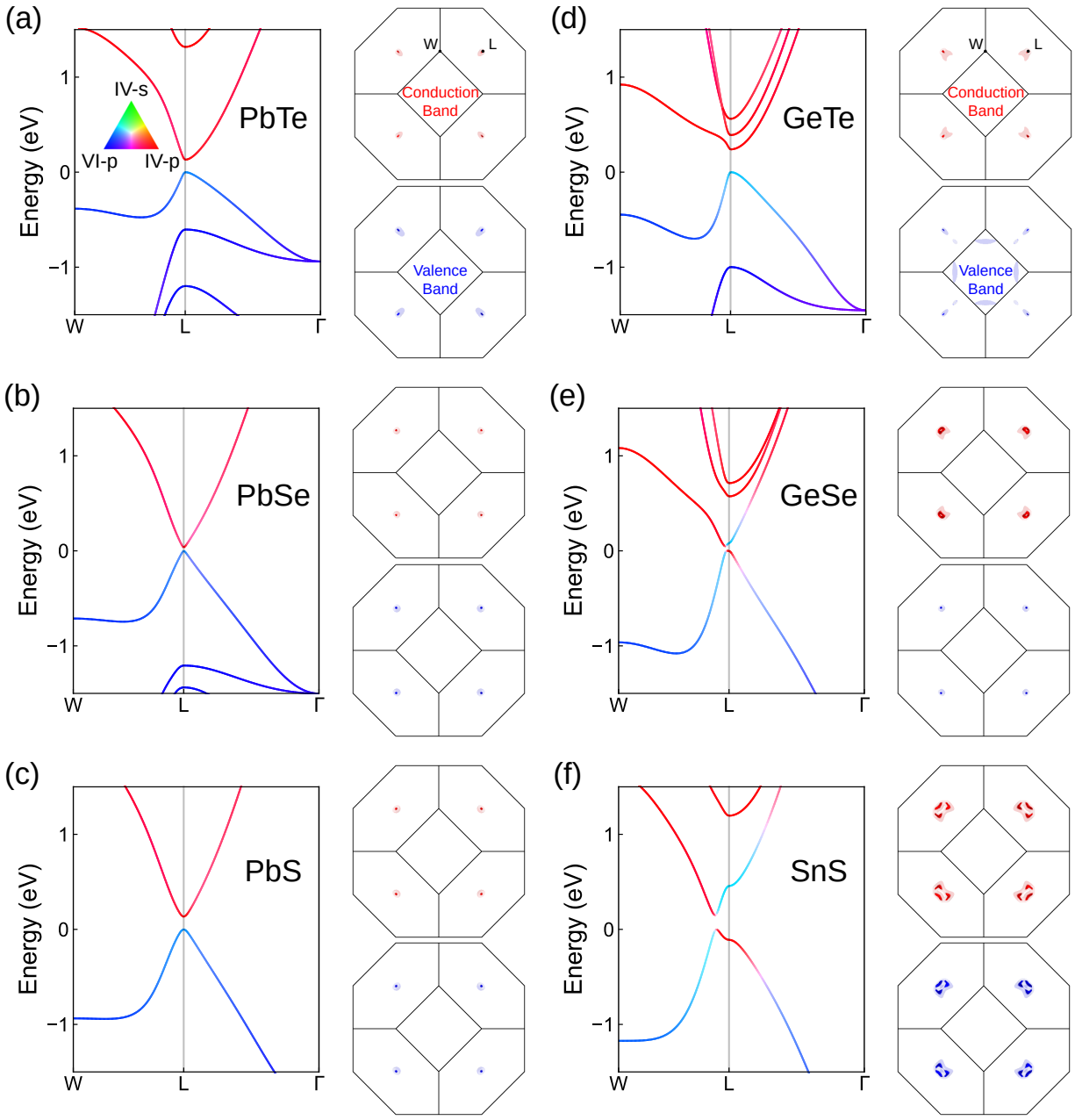

Figure S1: Electronic bands of rock-salt (a) PbTe, (b) PbSe, (c) PbS, (d) GeTe, (e) GeSe, and (f) SnS. The bands are color-coded by contributions from the IV-s (green), IV-p (red), and VI-p (blue) atomic orbitals. The full-zone Fermi surfaces of the conduction (red) and valence (blue) bands are shown. Darker Fermi surface colors represent a constant-energy slice 10 meV away from the band edge, whereas lighter colors represent a slice 100 meV away from the band edge.

Close-Up View of the SnSe Fermi Surface

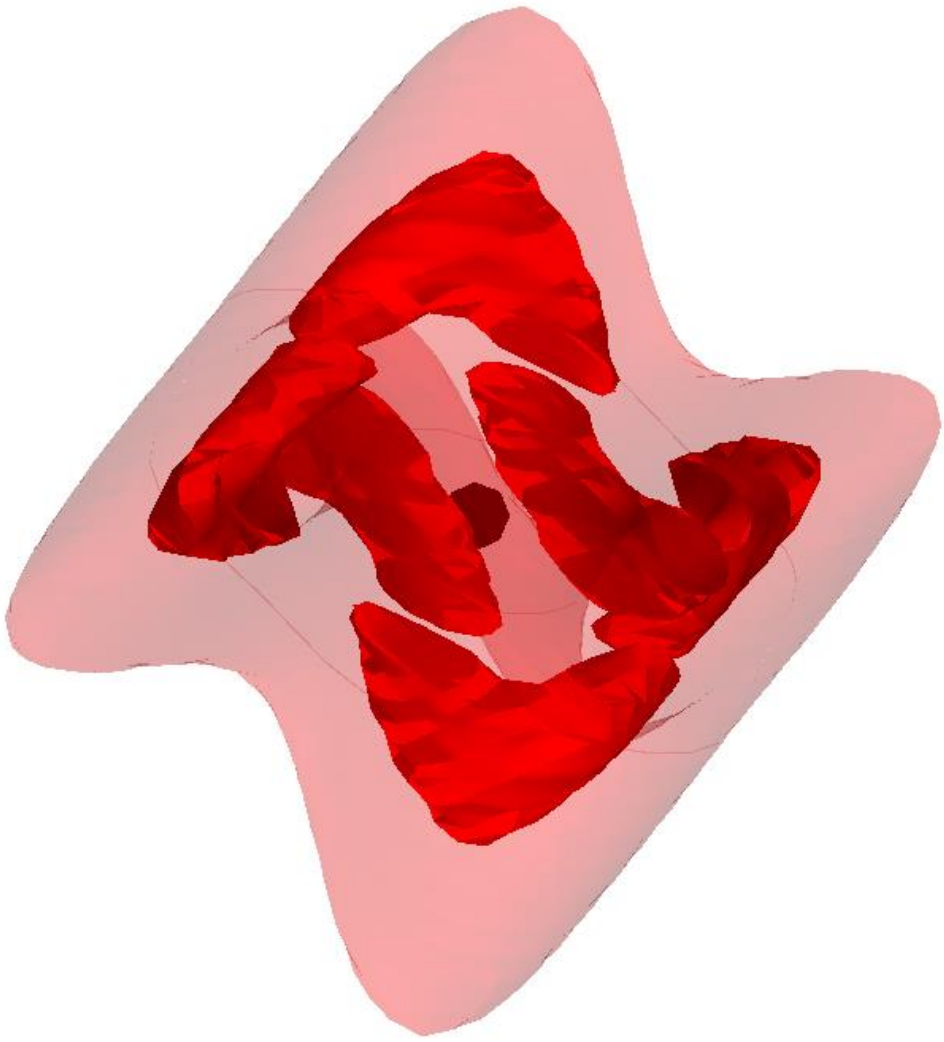

Figure S2: Fermi surface of SnSe around one of the L-points, shown as the black dot. The darker color represent a constant-energy slice 10 meV away from the band edge, whereas the lighter color represent a slice 100 meV away from the band edge.

12 Carrier Pockets from $\bar{3}m$ Symmetry

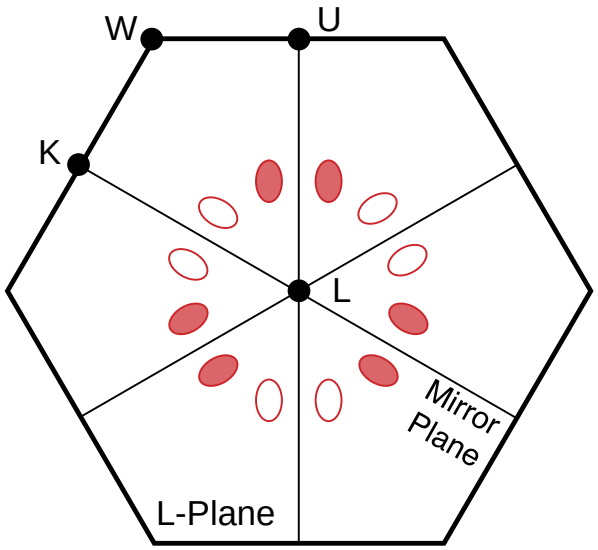

Figure S3: Twelve carrier pockets surrounding the L-point, which comply with the $\bar{3}m$ symmetry of the L-point. The filled and unfilled carrier pockets are located on opposite sides of the L-plane. This arrangement is distinct from the six-carrier pocket case (Figure 4b) since the carrier pockets do not lie on the mirror planes, which are shown as solid lines passing through the L-point.