

Electronic Supplementary Material (ESI) for RSC Advances

First Principles Study on Structural, Electronic and Optical Properties of $\text{HfS}_{2(1-x)}\text{Se}_{2x}$ and $\text{ZrS}_{2(1-x)}\text{Se}_{2x}$ Ternary Alloys

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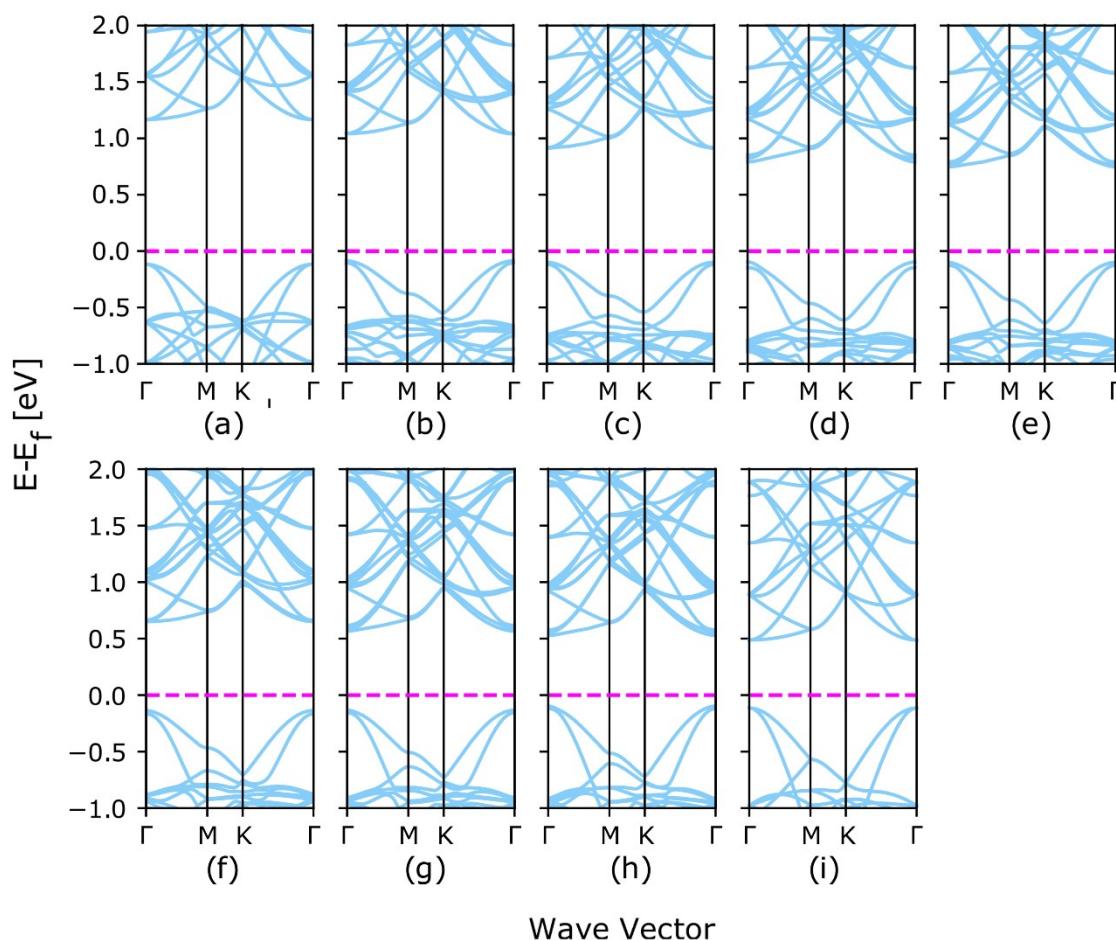


Fig. S1 Folded electronic band-structures of (a) $\text{Hf}_{16}\text{S}_{32}$ (b) $\text{Hf}_{16}\text{S}_{28}\text{Se}_4$ (c) $\text{Hf}_{16}\text{S}_{24}\text{Se}_8$ (d) $\text{Hf}_{16}\text{S}_{20}\text{Se}_{12}$ (e) $\text{Hf}_{16}\text{S}_{16}\text{Se}_{16}$ (f) $\text{Hf}_{16}\text{S}_{12}\text{Se}_{20}$ (g) $\text{Hf}_{16}\text{S}_8\text{Se}_{24}$ (h) $\text{Hf}_{16}\text{S}_4\text{Se}_{28}$ (i) $\text{Hf}_{16}\text{Se}_{32}$ in a $4 \times 4 \times 1$ supercell.

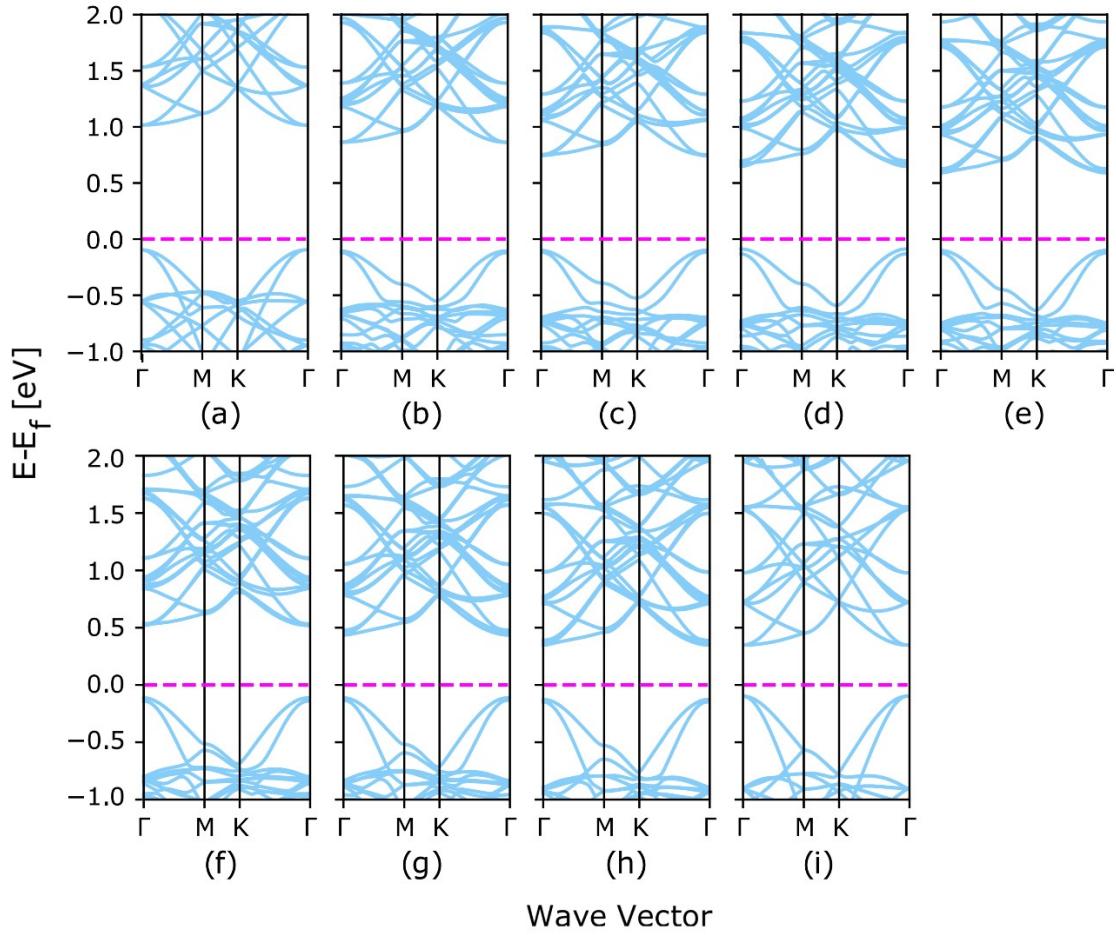


Fig. S2 Folded electronic band-structures of (a) $\text{Zr}_{16}\text{S}_{32}$ (b) $\text{Zr}_{16}\text{S}_{28}\text{Se}_4$ (c) $\text{Zr}_{16}\text{S}_{24}\text{Se}_8$ (d) $\text{Zr}_{16}\text{S}_{20}\text{Se}_{12}$ (e) $\text{Zr}_{16}\text{S}_{16}\text{Se}_{16}$ (f) $\text{Zr}_{16}\text{S}_{12}\text{Se}_{20}$ (g) $\text{Zr}_{16}\text{S}_8\text{Se}_{24}$ (h) $\text{Zr}_{16}\text{S}_4\text{Se}_{28}$ (i) $\text{Zr}_{16}\text{Se}_{32}$ in a $4 \times 4 \times 1$ supercell.

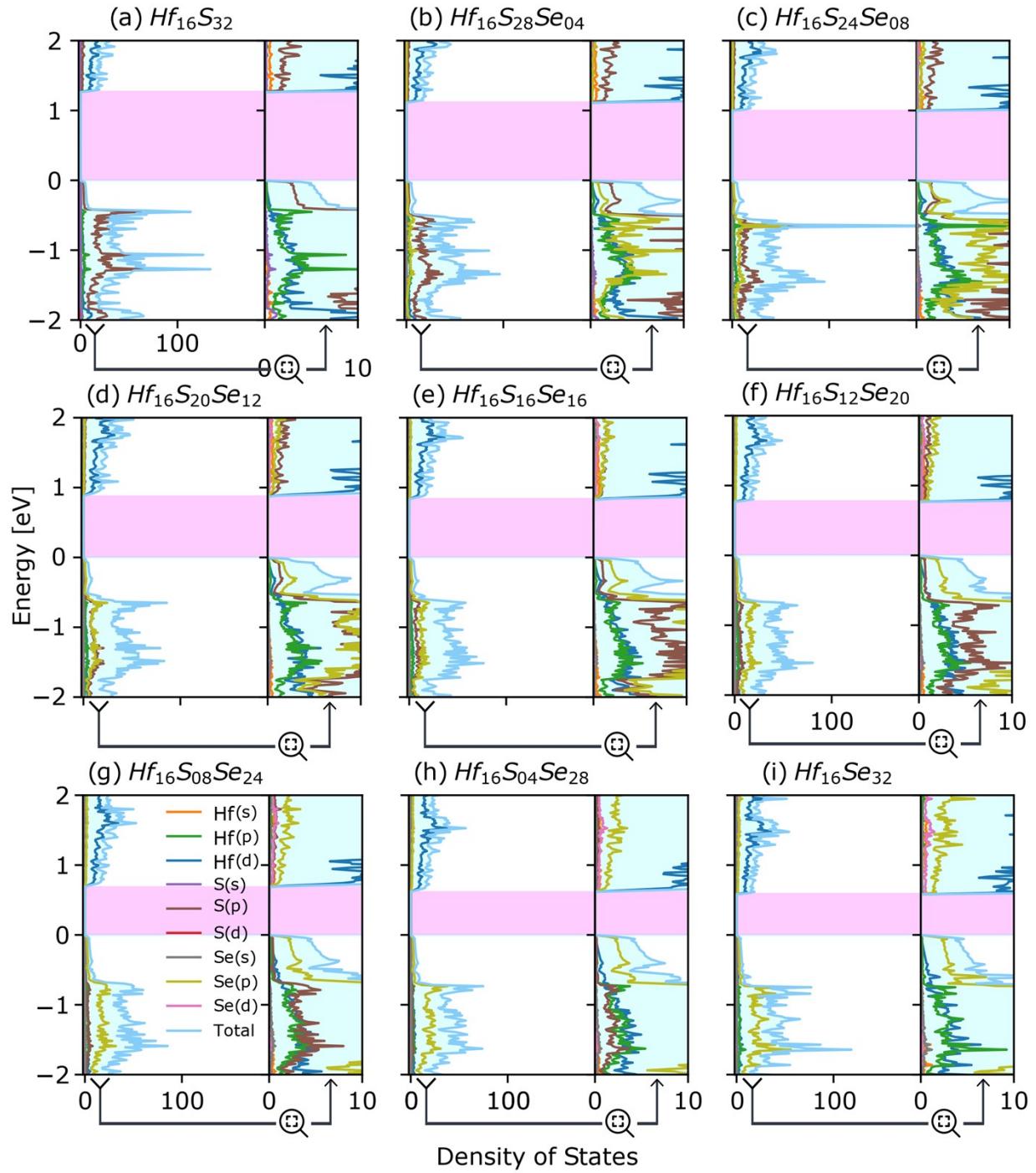


Fig. S3 The total and partial density of states (DOS) of (a) $Hf_{16}S_{32}$ (b) $Hf_{16}S_{28}Se_4$ (c) $Hf_{16}S_{24}Se_8$ (d) $Hf_{16}S_{20}Se_{12}$ (e) $Hf_{16}S_{16}Se_{16}$ (f) $Hf_{16}S_{12}Se_{20}$ (g) $Hf_{16}S_8Se_{24}$ (h) $Hf_{16}S_4Se_{28}$ (i) $Hf_{16}Se_{32}$.

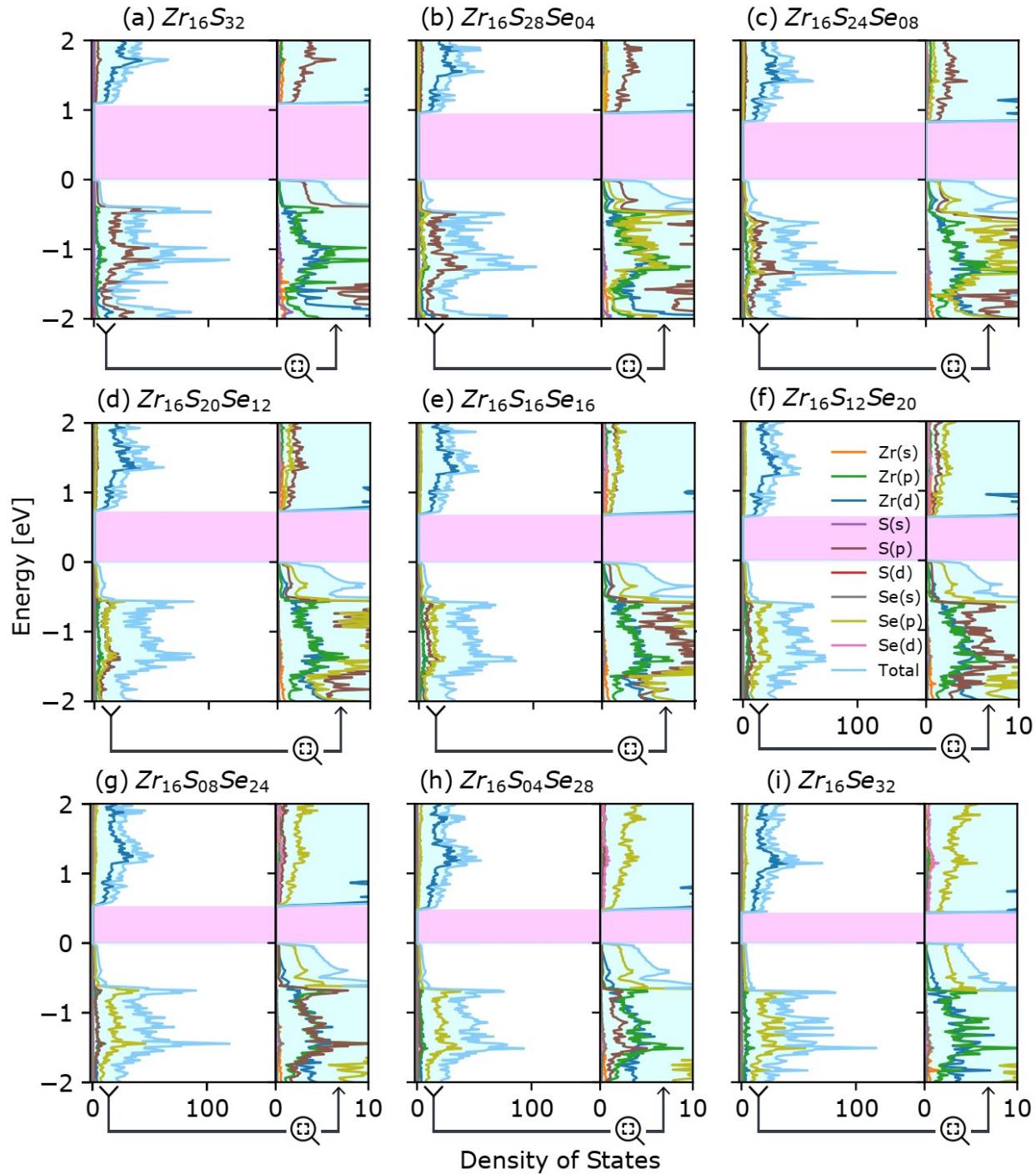


Fig. S4 The total and partial density of states (DOS) of (a) $Zr_{16}S_{32}$ (b) $Zr_{16}S_{28}Se_4$ (c) $Zr_{16}S_{24}Se_8$ (d) $Zr_{16}S_{20}Se_{12}$ (e) $Zr_{16}S_{16}Se_{16}$ (f) $Zr_{16}S_{12}Se_{20}$ (g) $Zr_{16}S_8Se_{24}$ (h) $Zr_{16}S_4Se_{28}$ (i) $Zr_{16}Se_{32}$.