Supporting information

for

\(\sigma\)-antibonding between valence s-orbitals as a primary cause for band gaps in compounds of diamond-like structures

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Figure S.1. COHP plot calculated for the Au-Sn bond on the basis of first principles TB-LMTO calculations for ScAuSn.
Figure S.2. Dispersion relations of the bands around the Fermi level calculated for (a) CaAuBi and (b) YAuPb by using the self-consistent full-potential linearized augmented-plane-wave method embodied in the WIEN2k code. The fat band representation is given for the valence s-orbital contributions of all the atoms.
Figure S.3. Schematic representation of the $\sigma$-antibonding orbital of AML at $\Gamma$, which is made up of the valence ns orbitals of M and L, around each electropositive atom A (a yellow circle) located at the center of an M$_4$ tetrahedron (shaded large circles) and an L$_6$ octahedron (unshaded medium circles). The ns orbitals of the M atoms make antibonding interactions with those of the adjacent L atoms such that the four ns orbitals of the M$_4$ tetrahedron make a group orbital of $a_1$ symmetry, and those of the L$_6$ octahedron a group orbital of $a_{1g}$ symmetry.