Supporting Information

Hypervalent Bismuthides La$_3$MBi$_5$ ($M =$ Ti, Zr, Hf) and Related Antimonides: Absence of Superconductivity

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Figure S1. Comparison of XRD patterns for \( \text{La}_3\text{Ti(\text{Bi}_{1-x}\text{Sb}_x)}_5 \). There are several amounts of \( \text{La(\text{Bi,Sb})} \) and unindexed impurity phases.
Figure S2. Low temperature magnetic susceptibility for La₅Ti(Bi₁₋ₓSbₓ)₅ at 20 Oe with zero-field-cooled and field-cooled processes.
Figure S3. (a) Calculated band structure for La$_3$TiSb$_5$ where Γ = (0,0,0), K = (1/3,1/3,0), M = (1/2,0,0),
A = (0,0,1/2), L = (1/2,0,1/2), and H = (1/3,1/3,1/2) in the Brillouin Zone. (b) Total and projected
density of states for La$_3$TiSb$_5$. Fermi level $E_F = 0$ eV.
Figure S4. Calculated Fermi surface and its four separate components for (a) La$_3$TiBi$_5$ and (b) La$_3$TiSb$_5$. 
Figure S5. (a) Computed band structures for (a) La$_3$TiSb$_5$ and (b) La$_3$TiBi$_5$ with SOC.
Figure S6. Computed band structures for La$_3$ZrSb$_5$ (a) without and (b) with SOC and for La$_3$HfSb$_5$ (c) without and (d) with SOC.