SUPPLEMENTARY MATERIAL

Crystal structure, bonding and electronic structure of α- and β-Ir_2B_{3-x} compounds

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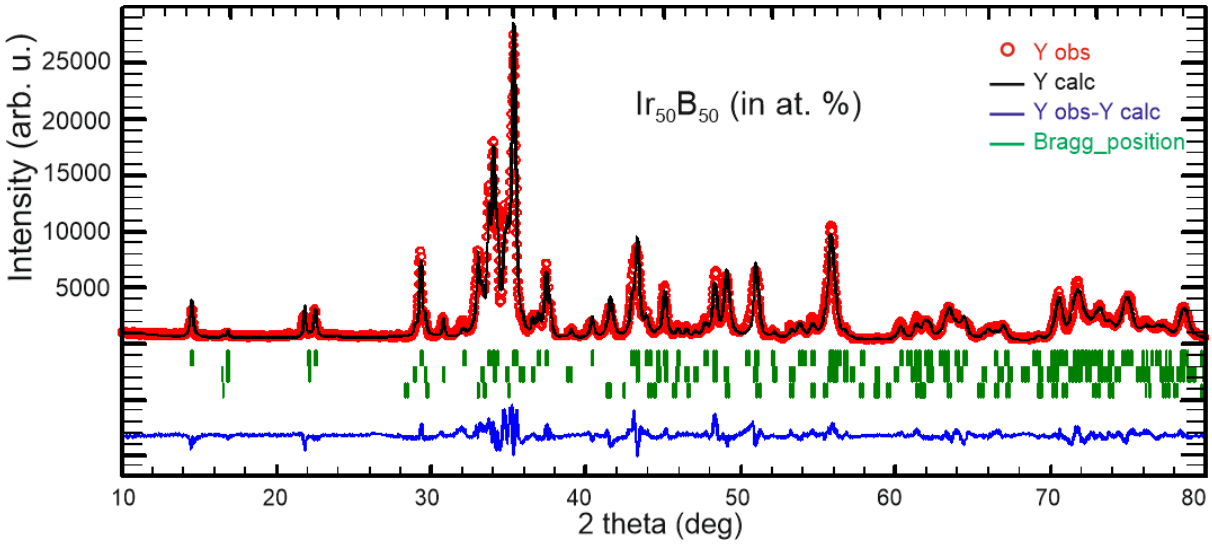

Figure S1. Powder X-ray diffraction pattern of ~$Ir_{50}B_{50}$ (in at. %) sample obtained from high-temperature synthesis. Upper row of *hkl* labels corresponds to *α*-Ir_3B_{2-x} (space group *C*2/*m*; a=10.5433(8) Å, b=2.8924(3) Å, c=6.0927(6) Å, β=91.052(6)º), middle row represents the *β*-Ir_3B_{2-x} (space group *Pnma*; a=10.766(1) Å, b=2.8422(5) Å, c=6.0367(9) Å), lower row stands for the phase Ir_5B_4 (space group $I4_1/a$, a=6.2912(6) Å, c=10.256(1) Å). For Rietveld refinement, the structure models of *α*-Ir_2B_{3-x} (single crystal X-ray diffraction data; current work), Ir_3B_{2-x} [20] and *β*-Ir_2B_{3-x} (denoted as Ir_5B_4 in [23]) were applied. Crystal structure data of *β*-Ir_3B_{2-x} as obtained from Rietveld refinement of powder pattern of HTS sample: space group *Pnma*; a=10.766(1) Å, b=2.8422(5) Å, c=6.0367(9) Å; Ir1 in 4*c*, *x*=0.8539(8), *y*=¼, *z*=0.352(1), Ir2 in 4*c*, *x*=0.5981(8), *y*=¼, *z*=0.274(1), B1 in 4*c*, *x*=0.5713, *y*=¾, *z*=0.5280; B2 in 4*c*, *x*=0.8010, *y*=¾, *z*=0.0970; B3 in 4*c*, x=0.0080, *y*=¼, *z*=0.5570. Atom coordinates of boron atoms were fixed during refinement.

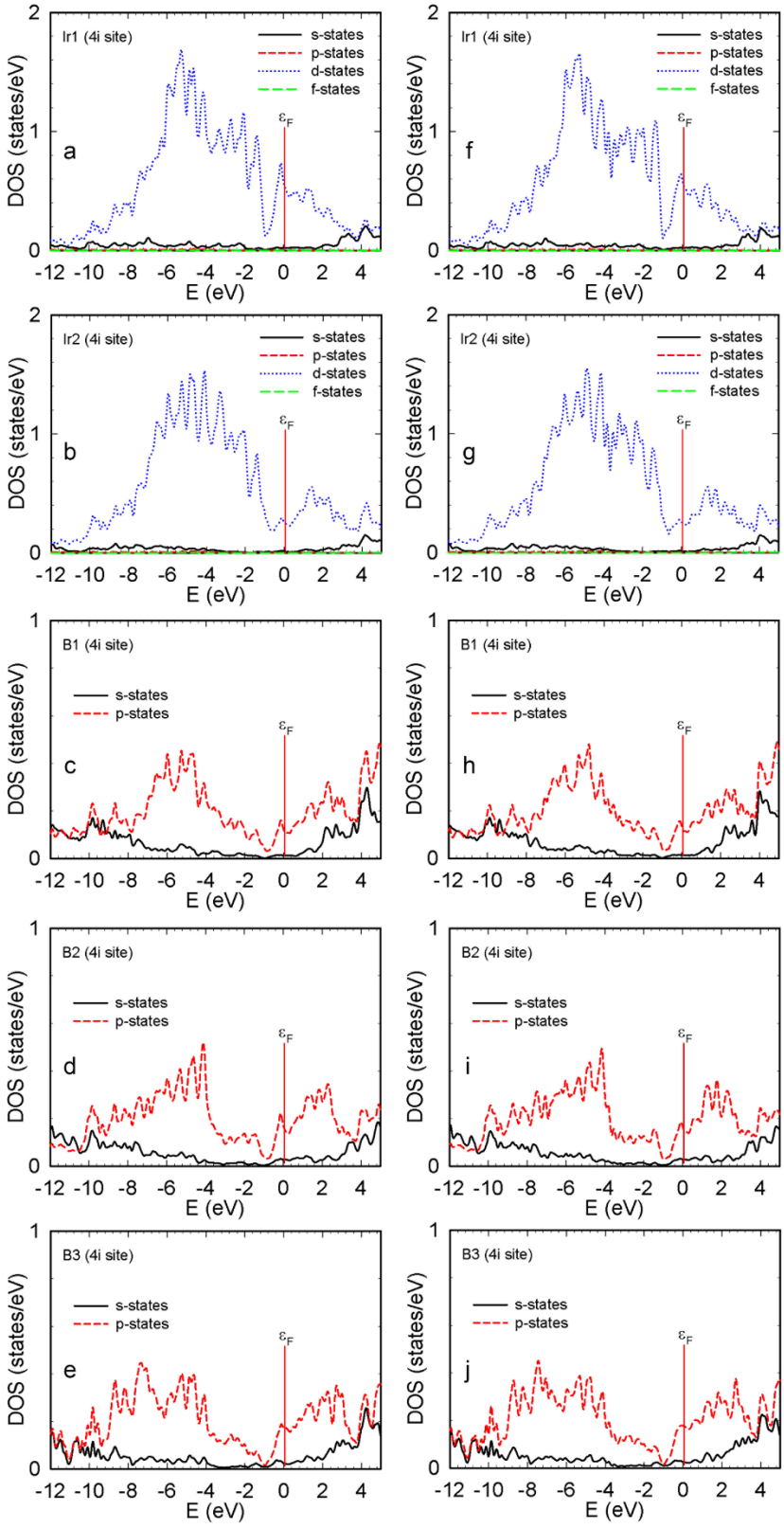

Figure S2. Distribution of partial (per one atom) density of states in α-Ir_2B_{3-x} without (a, b, c, d,e) and with (f, g, h, i, j) SOC.

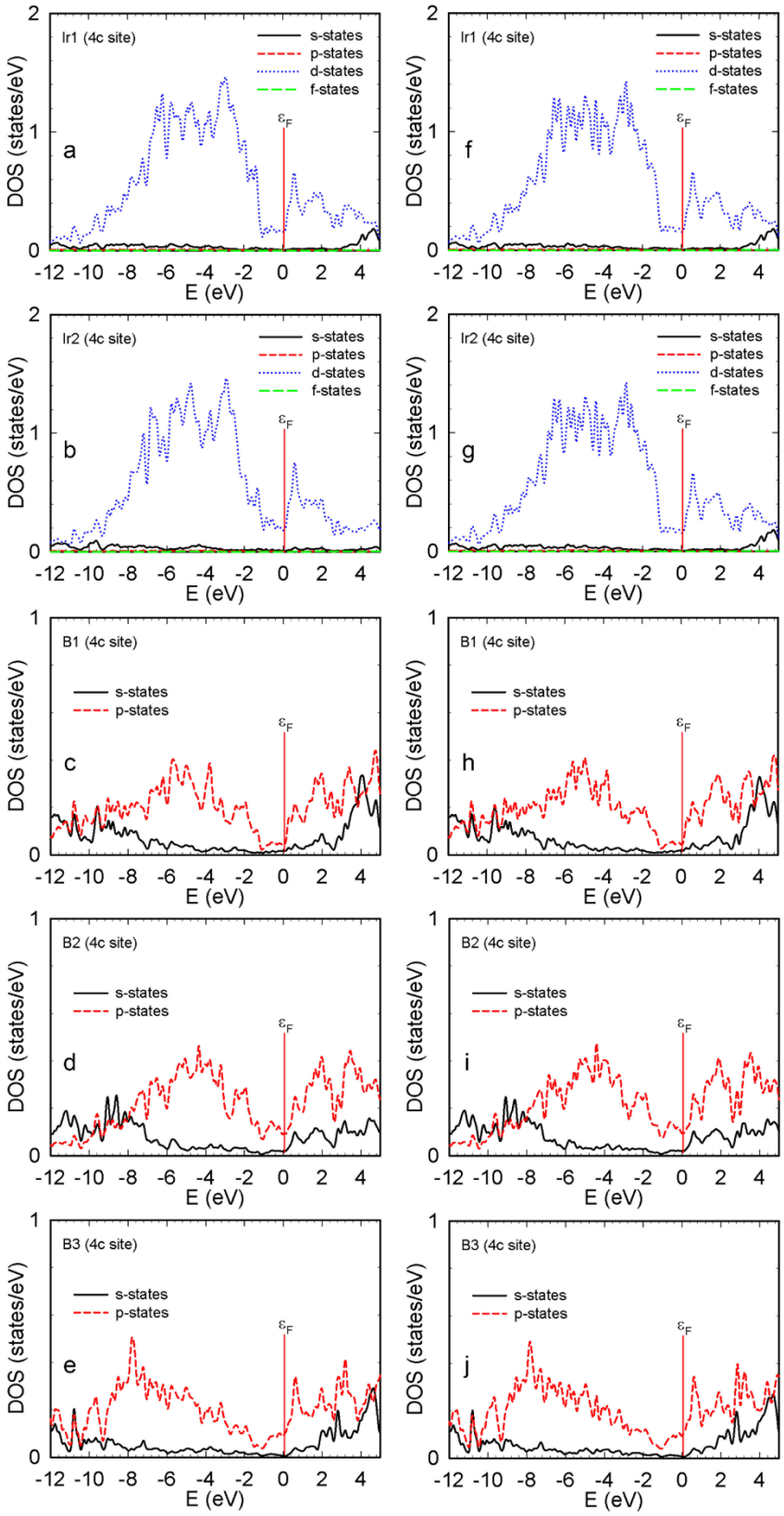

Figure S3. Distribution of the partial (per one atom) density of states in β-Ir_2B_{3-x} without (a, b, c, d,e) and with (f, g, h, i, j) SOC.

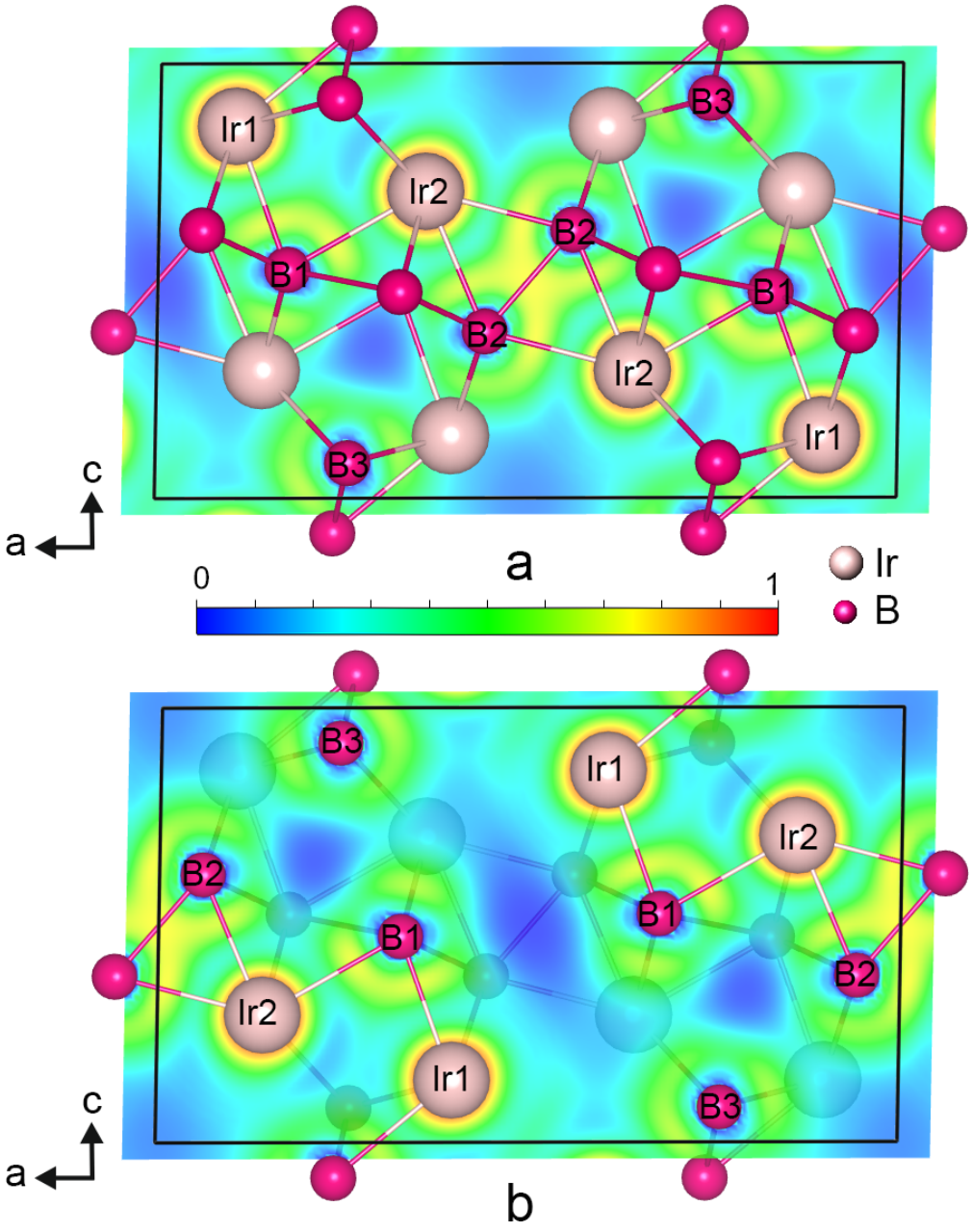

Figure S4. Sections of calculated electron localization function in α-Ir_2B_{3-x} structure within the (010) (a) and (020) (b) planes. Some atoms are located above (a) and below (b) the planes.

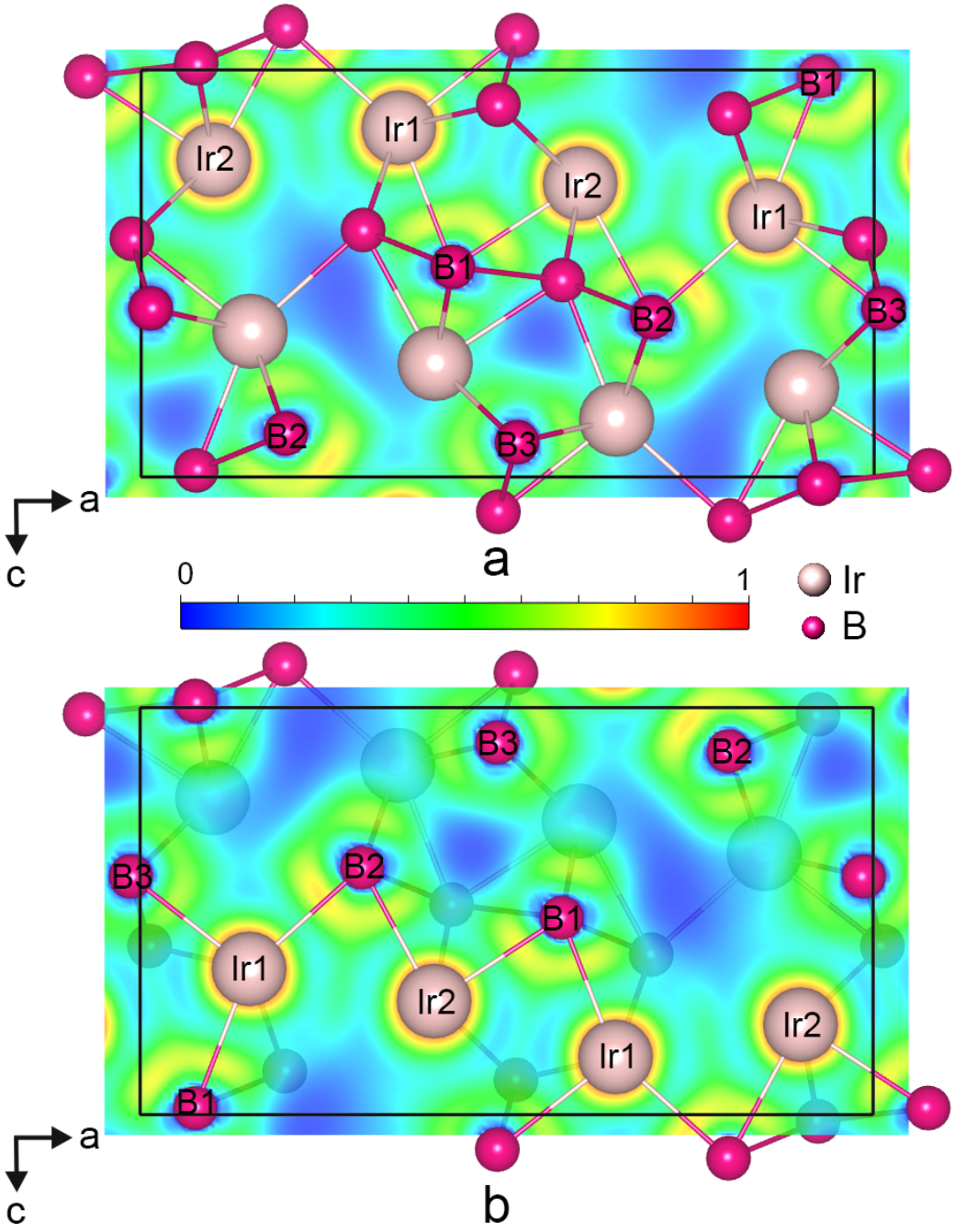

Figure S5. Sections of calculated electron localization function in β-Ir_2B_{3-x} structure within the (040) (a) and (080) (b) planes. Some atoms are located above (a) and below (b) the planes.

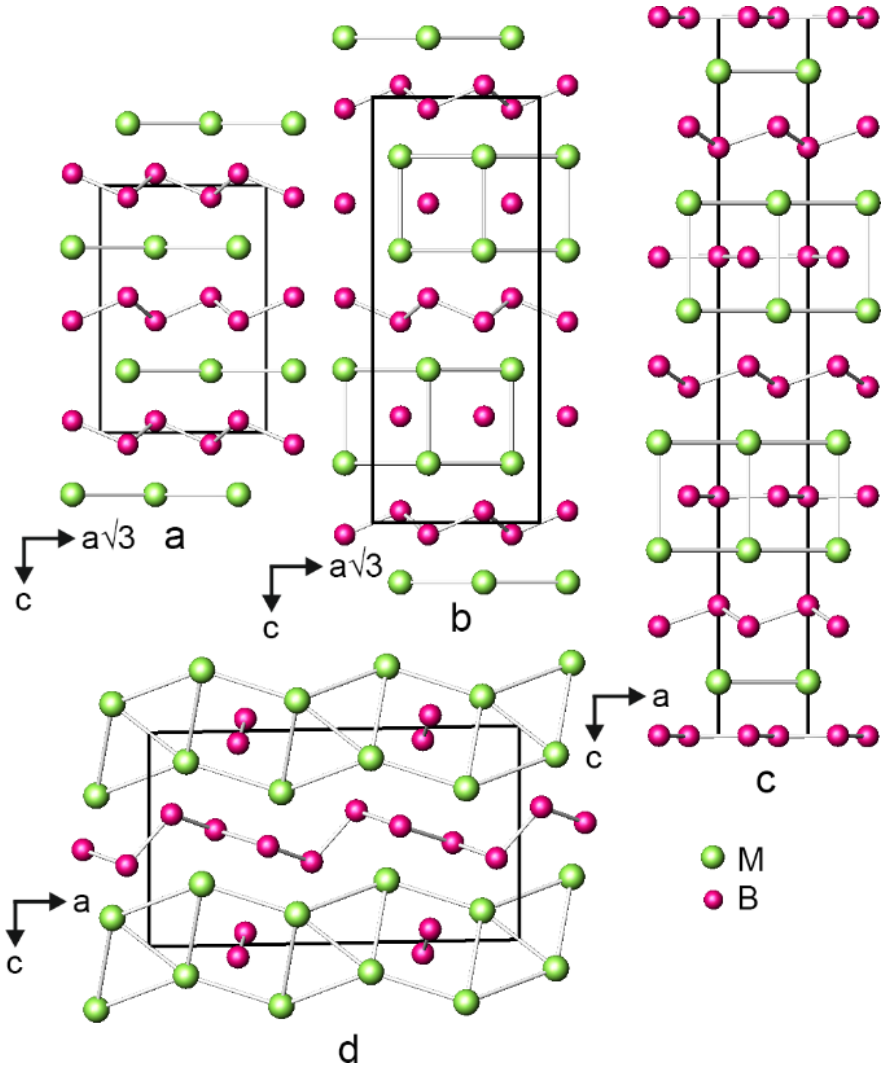

Figure S6. Crystal structures of ReB_2 (a), Ru_2B_3 (b), Mo_2B_4 (c) and α-Ir_2B_{3-x} (d).