Supplementary Material

The crystal structures, phase stabilities, electronic structures and bonding features of iridium borides from first-principles calculations

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Table S1 Structural information for the lowest energy phases for each components considered in the Ir−B binary system under ambient pressure.

Phase	Space group	Lattice parameters (Å, ◦)	Atom	Atomic coordinates (fractional)		
Ir_3B	*P*–6*m*2	*a*=2.794, *b*=2.792 *c*=7.513, *γ*=120	Ir(1f)	0.66667	0.33333	0.50000
			Ir(2h)	0.33333	0.66667	0.19345
			B(1e)	0.66667	0.33333	0.00000
Ir_2B	$P2_1/m$	*a*=5.699, *b*=2.803, *c*=4.736, *β*=80.720	Ir(2e)	0.97286	0.25000	0.76544
			Ir(2e)	0.52023	0.75000	0.23781
			B(2e)	0.75929	0.25000	0.41058
Ir_3B_2	*C*2/*m*	*a*=7.500, *b*=2.860, *c*=8.605, *β*=139.619	Ir(4i)	0.33331	0.00000	0.33495
			Ir(2a)	0.00000	0.00000	0.00000
			B(4i)	0.61554	0.00000	0.27856
Ir_4B_3	*Fmm*2	*a*=5.659, *b*=5.731, *c*=10.020	Ir(8d)	0.24894	0.00000	0.33235
			Ir(8b)	0.25000	0.25000	0.07929
			B(8c)	0.00000	0.25608	0.24163
			B(4a)	0.00000	0.00000	0.00000
Ir_5B_4	$P6_3/mmc$	*a*=3.521, *b*=3.521, *c*=18.957, *γ*=120	Ir(4f)	0.33333	0.66667	0.04790
			Ir(4e)	0.00000	0.00000	0.14924
			Ir(2c)	0.33333	0.66667	0.25000
			B(4f)	0.66667	0.33333	0.07907
			B(4f)	0.66667	0.33333	0.19462
IrB	$P2_1/m$	*a*=6.722, *b*=3.924, *c*=3.556, *β*=98.705	Ir(2e)	0.13814	0.25000	0.87934
			Ir(2e)	0.63715	0.25000	0.37912
			B(2e)	0.59694	0.25000	0.69884
			B(2e)	0.09582	0.25000	0.19876
Ir_4B_5	*Cm*	*a*=10.623, *b*=2.902, *c*=12.373, *β*=149.737	Ir(2a)	0.74463	0.00000	0.84784
			Ir(2a)	0.00000	0.00000	0.00000
			Ir(2a)	0.54485	0.00000	0.57077
			Ir(2a)	0.28472	0.00000	0.42031
			B(2a)	0.08389	0.00000	0.32761
			B(2a)	0.82194	0.00000	0.17625
			B(2a)	0.19934	0.00000	0.09735
			B(2a)	0.46237	0.00000	0.25205
			B(2a)	0.38533	0.00000	0.75904
Ir_3B_4	*Pnma*	*a*=16.266, *b*=2.962, *c*=6.028	Ir(4c)	0.01934	0.25000	0.21009
			Ir(4c)	0.18546	0.25000	0.09055
			Ir(4c)	0.35150	0.25000	0.17166
			B(4c)	0.13486	0.25000	0.42561
			B(4c)	0.40715	0.25000	0.50234
			B(4c)	0.21497	0.75000	0.35015
			B(4c)	0.04250	0.75000	0.46665
Ir_2B_3	$P6_3/mmc$	*a*=3.124, *b*=3.124, *c*=12.184,	Ir(4f)	0.33333	0.66667	0.13893

		γ=120	B(4f)	0.33333	0.66667	0.96097
			B(2d)	0.33333	0.66667	0.75000
IrB_2	*C*2/*m*	*a*=7.422, *b*=2.856, *c*=5.898, β=67.353	Ir(4c)	0.61236	0.25000	0.24258
			B(4c)	0.39454	0.25000	0.50840
			B(4c)	0.59708	0.25000	0.91963
Ir_2B_5	*R*3*m*	*a*=2.976, *b*=2.976, *c*=24.747, γ=120	Ir(3a)	0.66667	0.33333	0.97776
			Ir(3a)	0.66667	0.33333	0.16843
			B(3a)	0.66667	0.33333	0.07259
			B(3a)	0.66667	0.33333	0.25611
			B(3a)	0.33333	0.66667	0.04263
			B(3a)	0.33333	0.66667	0.10614
			B(3a)	0.33333	0.66667	0.22454
IrB_3	*Pnma*	*a*=9.825, *b*=3.145, *c*=4.546	Ir(4c)	0.10600	0.25000	0.35280
			B(4c)	0.95110	0.25000	0.01260
			B(4c)	0.32320	0.25000	0.19080
			B(4c)	0.28850	0.25000	0.59090
			B(4c)	0.28850	0.25000	0.59090

Table S2 Calculated elastic compliance constants S_{ij} for the six considered structures in the Ir-B binary system.

Phase	Ir_2B	Ir_3B_2	Ir_4B_3	IrB	Ir_4B_5	Ir_3B_4
Space Group	$P2_1/m$	$C2/m$	$Fmm2$	$P2_1/m$	Cm	$Pnma$
S_{11}	0.002162	0.003216	0.001999	0.006793	0.002857	0.001935
S_{22}	0.002425	0.002630	0.002876	0.005339	0.002955	0.003126
S_{33}	0.004388	0.002964	0.003104	0.006640	0.002500	0.002260
S_{44}	0.006651	0.005877	0.011116	0.016247	0.013626	0.013343
S_{55}	0.041190	0.005598	0.010718	0.010759	0.006322	0.006765
S_{66}	0.016536	0.007860	0.008380	0.021858	0.015798	0.013192
S_{12}	–0.000419	–0.000888	–0.000425	–0.000873	–0.000800	–0.000375
S_{13}	–0.000510	–0.001311	–0.000658	–0.004120	–0.000929	–0.000405
S_{23}	–0.001344	–0.000542	–0.001251	–0.001426	–0.000588	–0.001127
S_{15}	0.000373	0.000566		–0.000749	–0.000684	
S_{25}	0.002713	–0.000456		0.002712	0.000839	
S_{35}	–0.009182	0.000072		0.001521	–0.000120	
S_{46}	–0.003480	–0.001001		0.014071	0.005929	

Table S3 The calculated ICOHP of solid α-B, $P2_1/m$-Ir_2B, $C2/m$-Ir_3B_2, $Fmm2$-Ir_4B_3, $P2_1/m$-IrB, Cm-Ir_4B_5, and $Pnma$-Ir_3B_4.

Phase	Space group	Bond length (Å)	ICOHP (eV)
B	$R-3m$	B-B[1]=1.67	–7.72
		B-B[2]=1.80	–4.62
		B-B[3]=1.74	–4.81
		B-B[4]=2.00	–3.47
Ir_2B	$P2_1/m$	Ir-B[1]=2.14	–2.89
		Ir-B[2]=2.20	–2.55
Ir_3B_2	$C2/m$	Ir-B[1]=2.15	–3.00
		Ir-B[2]=2.19	–2.86
Ir_4B_3	$Fmm2$	Ir-B=2.16	–3.05
IrB	$P2_1/m$	Ir-B[1]=2.11	–3.01
		Ir-B[2]=2.17	–3.10
Ir_4B_5	Cm	Ir-B[1]=2.16	–2.98
		Ir-B[2]=2.17	–2.63
		Ir-B[3]=2.13	–2.58
		B-B[1]=1.89	–5.03
		B-B[2]=2.00	–3.93
		B-B[3]=2.12	–3.03
Ir_3B_4	$Pnma$	Ir-B[1]=2.17	–2.50
		Ir-B[2]=2.20	–2.28
		B-B[1]=2.02	–3.97
		B-B[2]=2.12	–3.08
		B-B[3]=2.06	–3.62

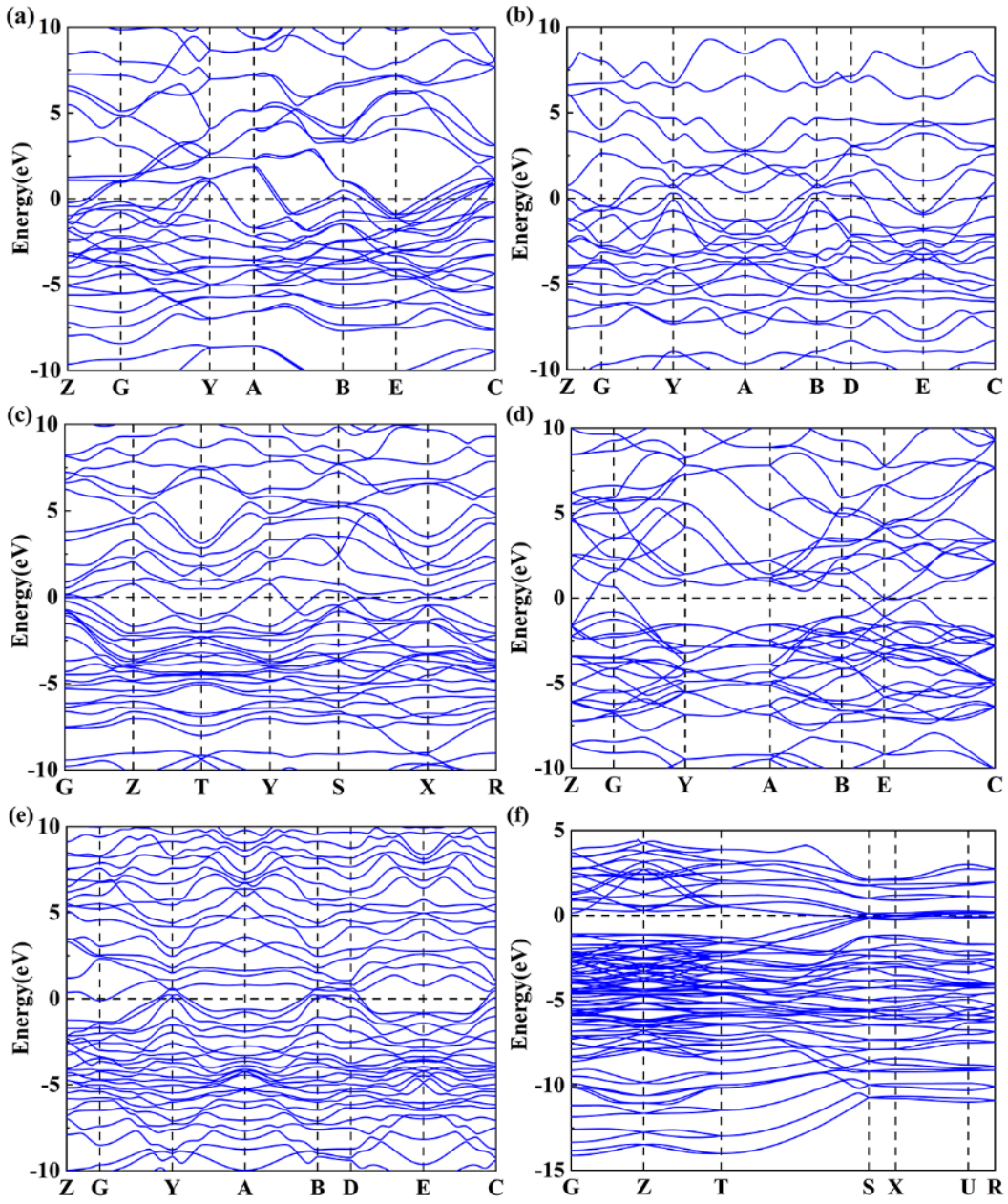

Fig. S1 Calculated electronic band structures for (a) $P2_1/m$–Ir_2B, (b) $C2/m$–Ir_3B_2, (c) $Fmm2$–Ir_4B_3 (d) $P2_1/m$–IrB, (e) Cm–Ir_4B_5 and (f) $Pnma$–Ir_3B_4 at atmospheric pressure.