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First principles investigation on chemical bonding of transition metal borides and carbides

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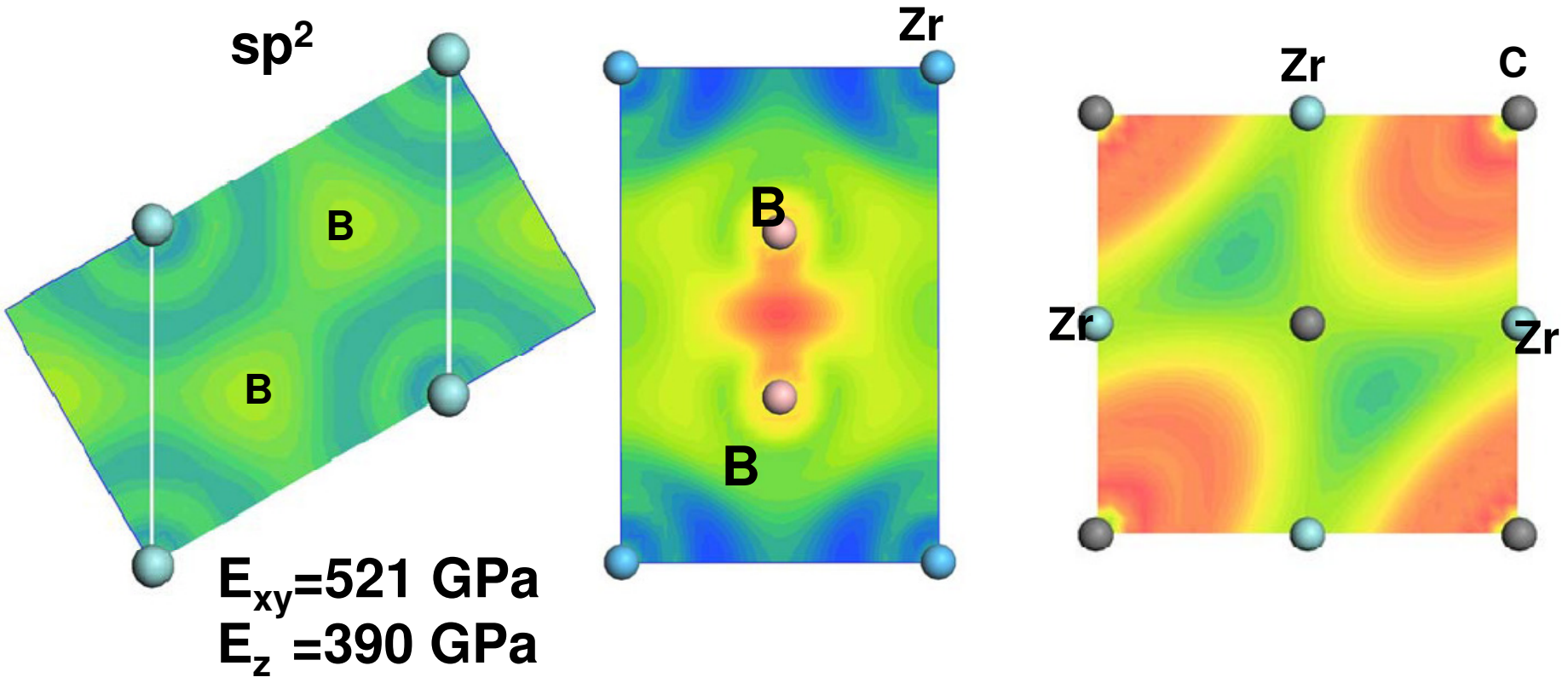
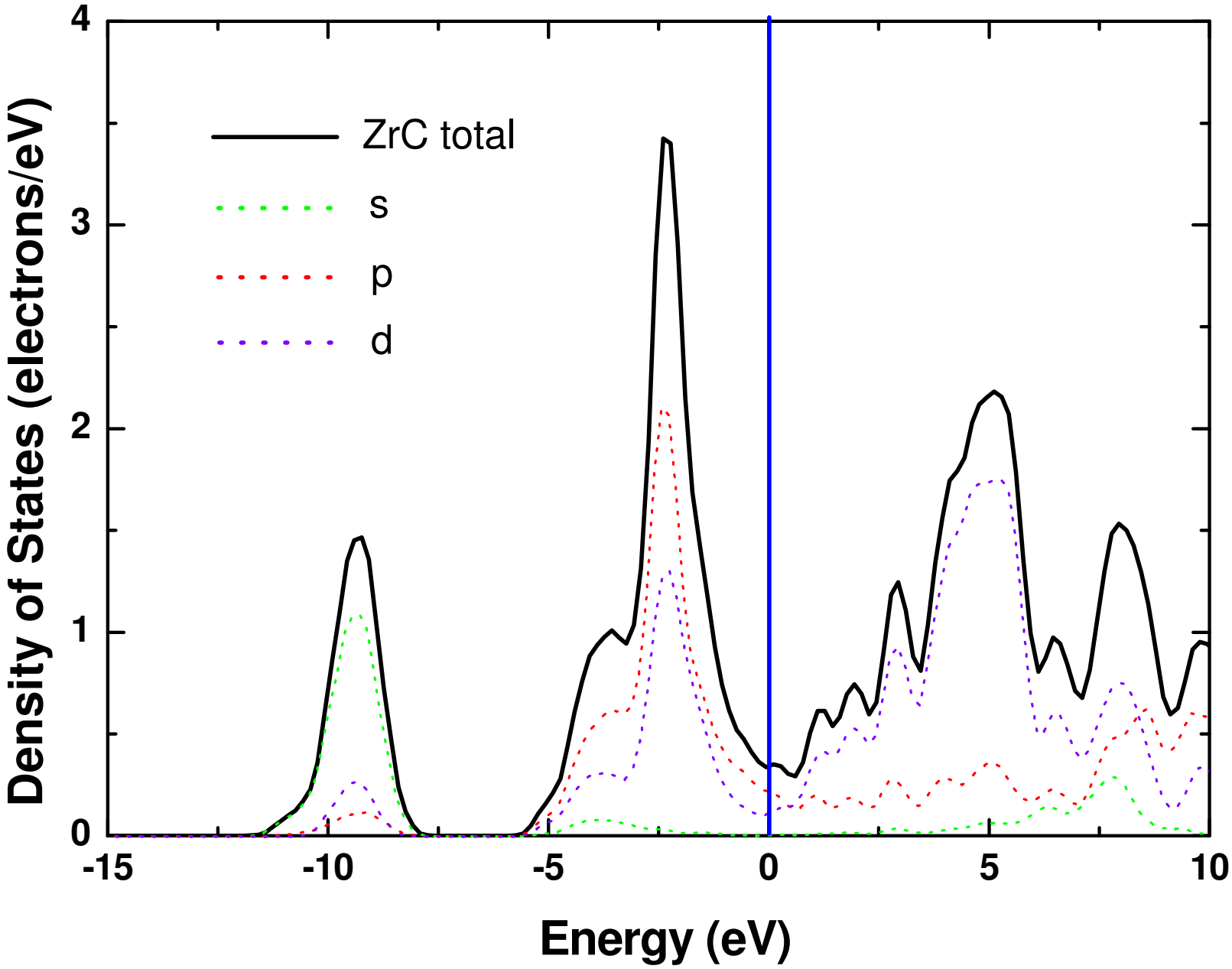
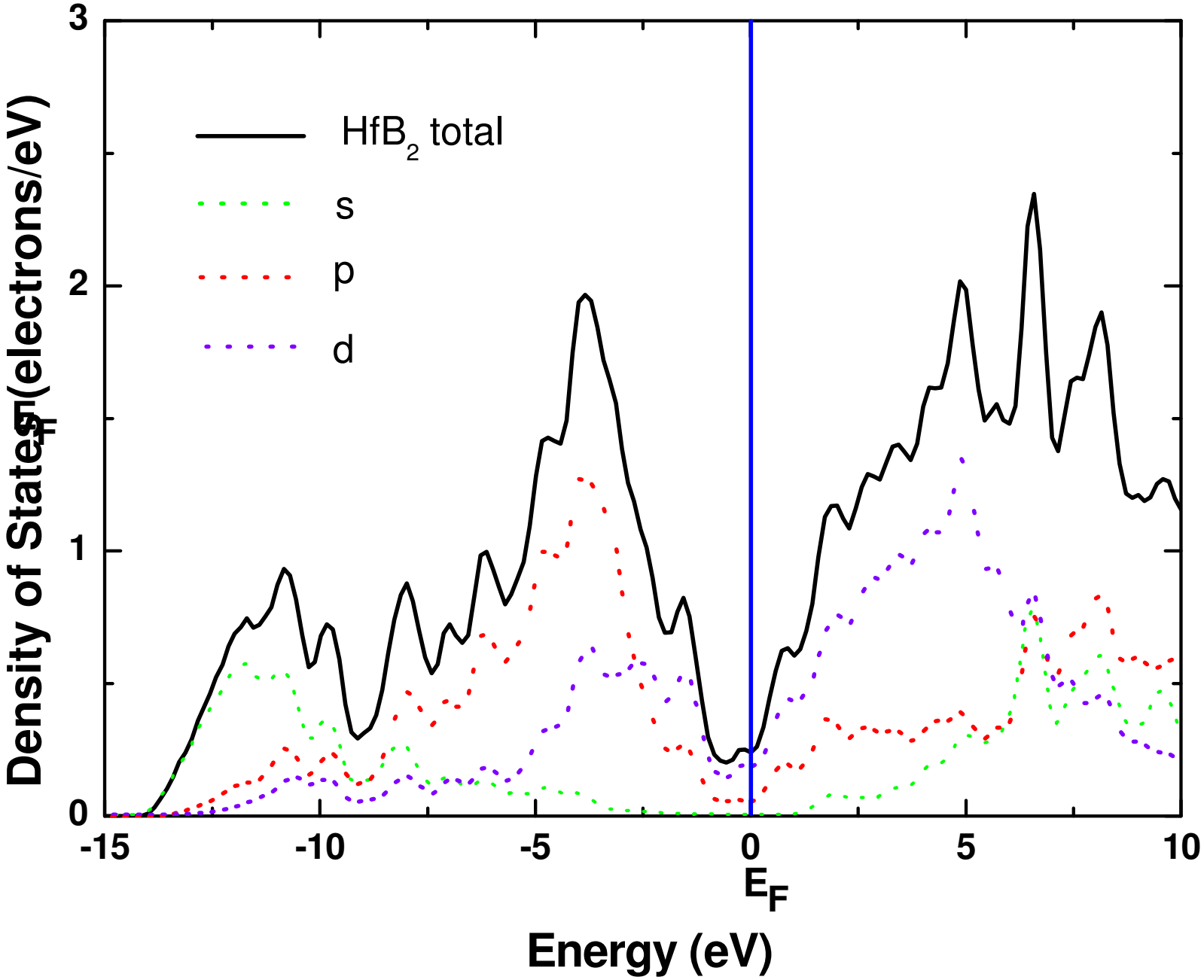



ZrC total
s
p
d
Density of States (electrons/eV)
Energy (eV)
0
1
2
3
4
-15
-10
-5
0
5
10


HfB2 total
s
p
d
Density of States (electrons/eV)
3
2
1
0
-15
-10
-5
0
5
10
EF
Energy (eV)

Elastic properties of transition metal carbides and borides

	Ex (GPa)	Ey (GPa)	Ez (GPa)	E (GPa)	B (GPa)	G (GPa)	G/E
ZrC	410.52	410.52	410.52	407	221.59	161.89	0.72
ZrB_2	521.10	521.10	390.43	523	238.31	230.98	0.96
HfB_2	537.51	537.51	403.73	542	261.35	232.71	0.89
NbB_2	522.86	522.86	387.75	525	288.87	219.79	0.76
TaB_2	486.25	486.25	354.00	480	299.63	169.74	0.56