Electronic Supplementary Material (ESI) for RSC Advances.

Metallic boro-carbides of A_2BC (A=Ti, Zr, Hf and W): A comprehensive theoretical study for thermo-mechanical and optoelectronic applications

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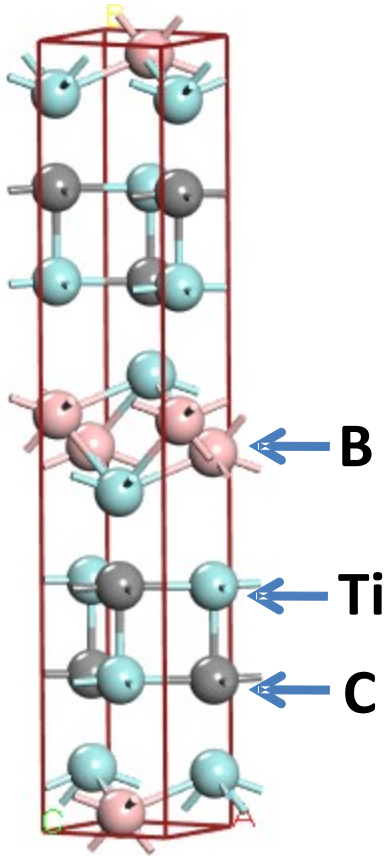

Fig. S1: The orthorhombic crystal structure of Ti_2BC compound.

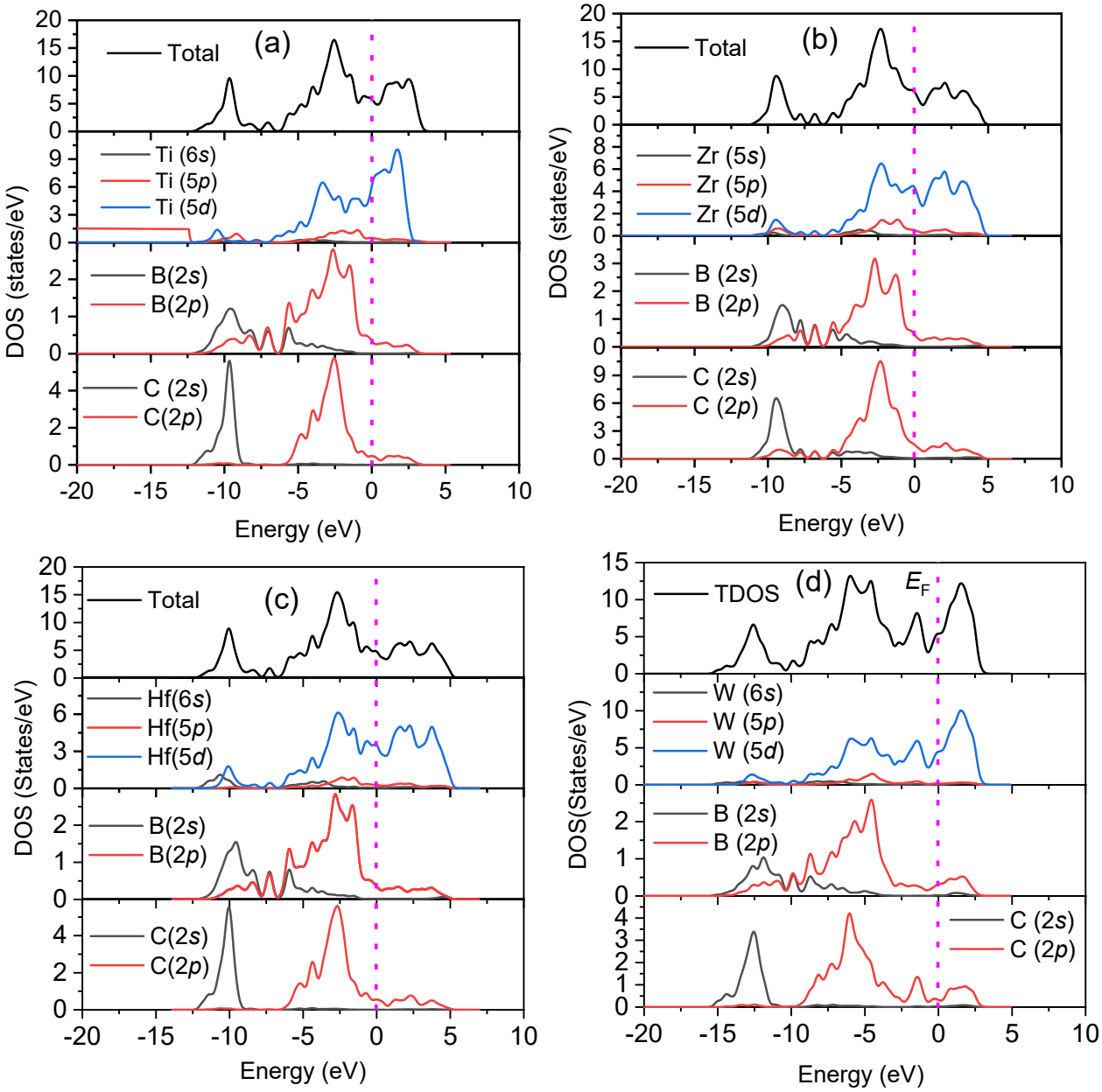

Fig. S2: Electronic partial density of states (DOS) for (a) Ti_2BC, (b) Zr_2BC, (c) Hf_2BC and (d) W_2BC compounds.

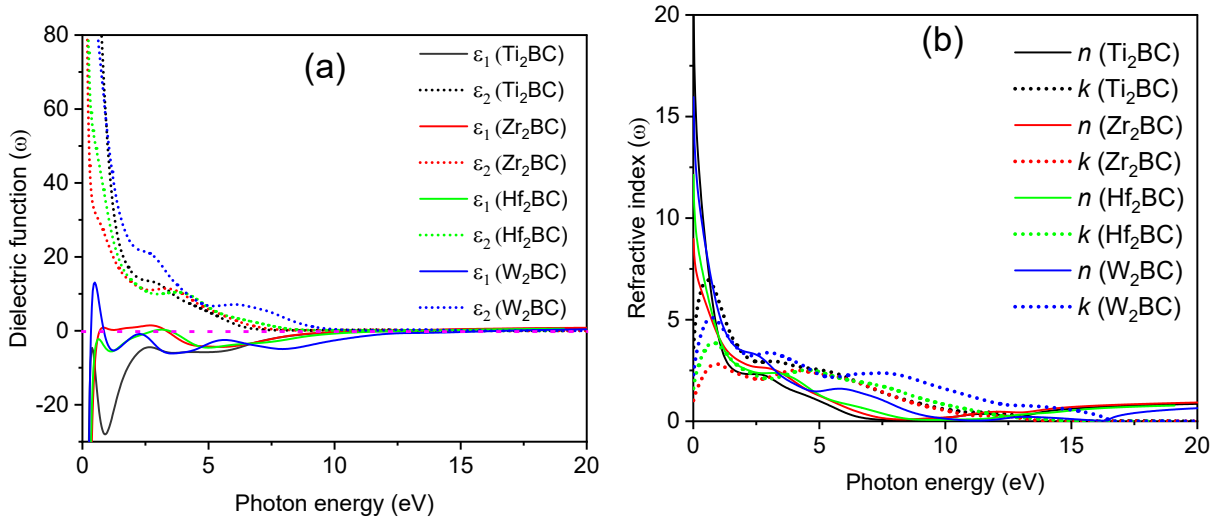

Fig. S3: Photon energy dependent (a) real part of dielectric function (ε_1) and imaginary part of dielectric function (ε_2), and (b) refractive index (n) and extinction coefficient (k) of A_2BC (A = Ti, Zr, Hf, and W) compounds.

Table S1: Lattice parameters (orthorhombic), *a*, *b* and *c* (all in Å), unit cell volume *V* (in Å^3) of A_2BC (A = Ti, Zr, Hf, and W) compounds and other available metallic boro-carbides compounds.

Compound	*a*	*b*	*c*	***V***	Ref.
Ti_2BC	3.165	17.587	3.089	169.11	This
	3.169	17.660	3.048	170.57	1
Zr_2BC	3.431	19.288	3.256	215.52	This
	3.437	19.473	3.273	219.08	1
Hf_2BC	3.420	19.127	3.256	213.04	This
	3.388	19.019	3.226	207.91	1
W_2BC	3.115	17.480	3.068	167.25	This
	3.125	17.578	3.086	169.54	1
V_2BC	2.999	16.770	2.956	148.70	1
	2.998	16.647	2.948	147.17	2
Nb_2BC	3.227	18.345	3.149	186.41	1
	3.224	18.239	3.141	184.71	2
Mo_2BC	3.119	17.580	3.082	169.01	1
	3.137	17.702	3.094	171.86	2
	3.094	17.768	3.091	169.93	3
	3.086	17.350	3.047	163.14	4
Ta_2BC	3.221	18.246	3.140	184.51	1
	3.267	18.445	3.180	191.69	2

Table S2: The calculated elastic stiffness constants C_{ij} (GPa) and Cauchy pressure (CP) (GPa) of A_2BC (A = Ti, Zr,Hf and W) compounds with other metallic boro-carbides.

Compound	C_{11}	C_{12}	C_{13}	C_{23}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	CP	Ref.
Ti_2BC	417	132	108	92	379	468	147	208	159	-15	This
Zr_2BC	374	124	96	96	325	408	121	175	130	+03	This
Hf_2BC	420	130	128	108	373	440	132	206	146	-02	This
W_2BC	563	257	240	258	532	572	184	291	189	+73	This
V_2BC	474	148	159	115	450	525	161	257	146	-13	2
Nb_2BC	482	154	156	134	488	504	140	251	130	+14	2
Mo_2BC	520	209	218	193	545	547	176	265	180	+33	2
	551	211	204	210	566	553	168	241	182	+43	3
Ta_2BC	503	157	181	153	468	528	134	258	125	+23	2

Table S3: Shear anisotropy factors (A_i) where i stand for 1, 2 and 3; bulk modulus (GPa) B_a, B_b and B_c along *a*-, *b*- and *c*-directions, respectively; anisotropy factors in compressibility (A_B) and shear moduli (A_G) (in %), and universal anisotropy index, A^U for A_2BC (A = Ti, Zr, Hf and W) compounds. The values for other metallic boro-carbides are given for comparison.

Compound	A_1	A_2	A_3	B_a	B_b	B_c	A_B	A_G	A^U	Ref.
Ti_2BC	0.87	1.25	1.195	685	561	691	0.234	1.54	0.16	This
Zr_2BC	0.82	1.30	1.15	624	503	622	0.22	1.47	0.15	This
Hf_2BC	0.87	1.38	1.10	716	564	698	0.23	1.31	0.14	This
W_2BC	1.12	1.98	1.30	1066	1015	1099	0.015	2.92	0.30	This
V_2BC	0.94	1.38	0.93	809	663	833	0.251	2.134	0.22	2
Nb_2BC	0.83	1.38	0.78	799	763	801	0.012	2.622	0.26	2
Mo_2BC	1.11	1.50	1.11	939	942	972	0.005	1.672	0.17	2
Ta_2BC	0.80	1.50	0.76	861	719	915	0.227	3.247	0.34	2

Table S4: Mulliken atomic and bond overlap populations of A_2BC (A = Ti, Zr, Hf and W) compounds. The EVC stands for effective valence charge.

		Atomic population						Bond overlap population			
Compound	Atom	s	p	d	Total	Charge (e)	EVC (e)	Bond	Bond number n^{μ}	Bond length d^{μ} (Å)	Bond population P^{μ}
Ti_2BC	C	1.48	3.24	0.00	4.72	-0.72	---	B-B	2	1.78777	1.47
	B	1.02	2.62	0.00	3.63	-0.63	---	C-Ti(I)	4	2.07903	0.25
	Ti	2.05	6.60	2.65	11.30	0.70	3.30	C-Ti(II)	4	2.10977	0.24
	Ti	2.13	6.62	2.59	11.34	0.66	3.34	C-Ti(III)	4	2.19435	1.51
								B-Ti(I)	4	2.32277	0.89
								B-Ti(II)	4	2.32689	-0.13
								Ti-Ti(I)	2	2.89955	-0.25
	C	1.50	3.29	0.00	4.79	-0.79	---	B-B	2	1.87731	1.42
Zr_2BC	B	1.05	2.59	0.00	3.63	-0.63	---	C-Zr(I)	4	2.29162	0.35
	Zr	2.13	6.47	2.68	11.29	0.71	3.29	C-Zr(II)	4	2.29402	0.30
	Zr	2.20	6.50	2.60	11.29	0.71	3.29	C-Zr(III)	4	2.36560	1.42
								B-Zr(I)	4	2.49658	-0.03
								B-Zr(II)	4	2.52756	0.94
								Zr-Zr	2	3.16471	-0.19
Hf_2BC	C	1.56	3.32	0.00	4.89	-0.89	---	B-B	2	1.9007	1.43
	B	1.18	2.64	0.00	3.81	-0.81	---	C-Hf(I)	4	2.27847	0.41
	Hf	0.35	-0.05	2.81	3.11	0.89	3.11	C-Hf(II)	4	2.30038	0.48
	Hf	0.43	0.02	2.73	3.19	0.81	3.19	C-Hf(III)	4	2.36171	1.51
								B-Hf(I)	4	2.49895	-0.12
								B-Hf(II)	4	2.50748	1.14
								Hf-Hf	2	3.12378	-0.24
W_2BC	C	1.38	3.30	0.00	4.68	-0.68	---	B-B	2	1.82386	1.20
	B	0.92	2.55	0.00	3.47	-0.47	---	C-W(I)	4	2.10329	0.14
	W	2.29	6.50	4.70	13.49	0.51	5.49	C-W(II)	4	2.16423	0.22
	W	2.36	6.49	4.51	13.36	0.64	5.36	C-W(III)	4	2.19304	1.54
								B-W(I)	4	2.31895	0.98
								W-W	2	2.95597	-0.49
								C-C	2	2.96839	-0.19

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