Supporting Information

Electronic structure, bonding characteristics, and mechanical behaviors of a new family of Si-containing damage-tolerant MAB phases M_5SiB_2 (M = IVB-VIB transition metals)

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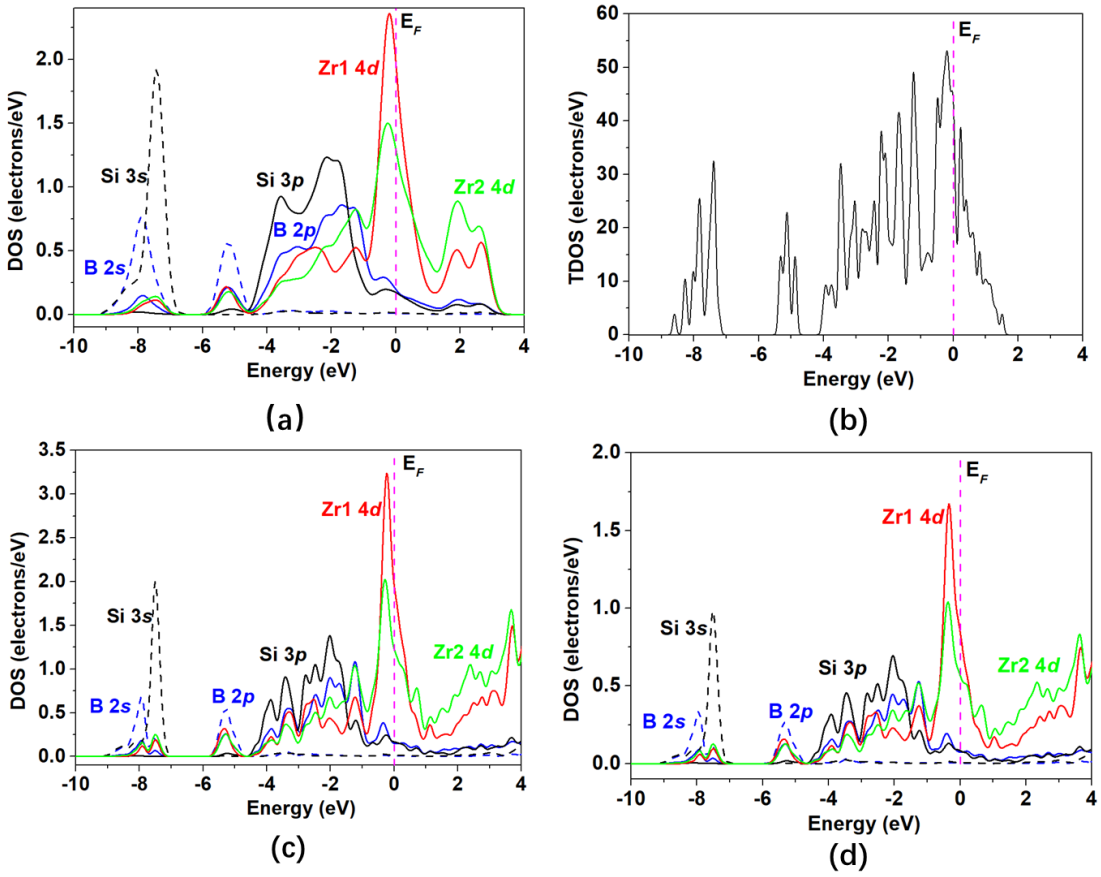

Figure S1 DOS of Zr_5SiB_2. (a) PDOS without SOC in this paper (a), (b)TDOS with SOC calculated with Norm-conserving pseudopotential. (c) PDOS without SOC calculated with the PAW pseudopotential. (d) PDOS with SOC calculated with the PAW pseudopotential.

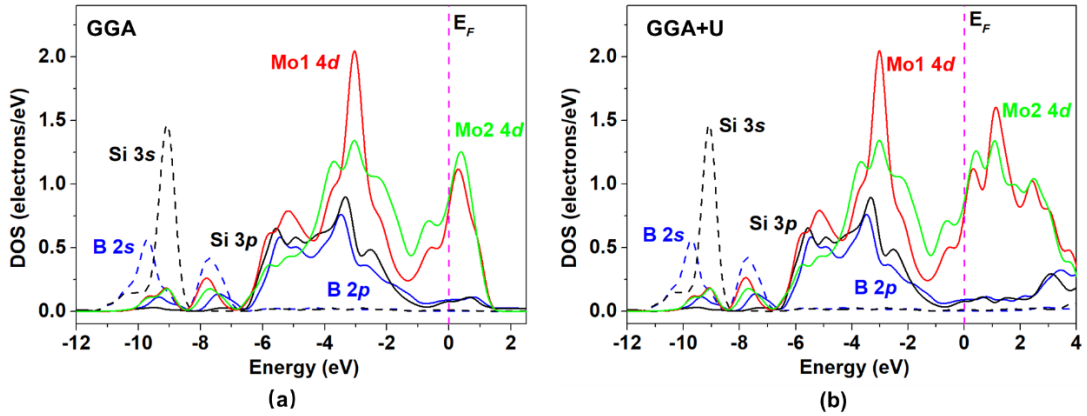

Figure S2 Projected density of states of Mo_5SiB_2 calculated with GGA (a) and GGA+U (b). A typical value of 2.5 eV was used for U

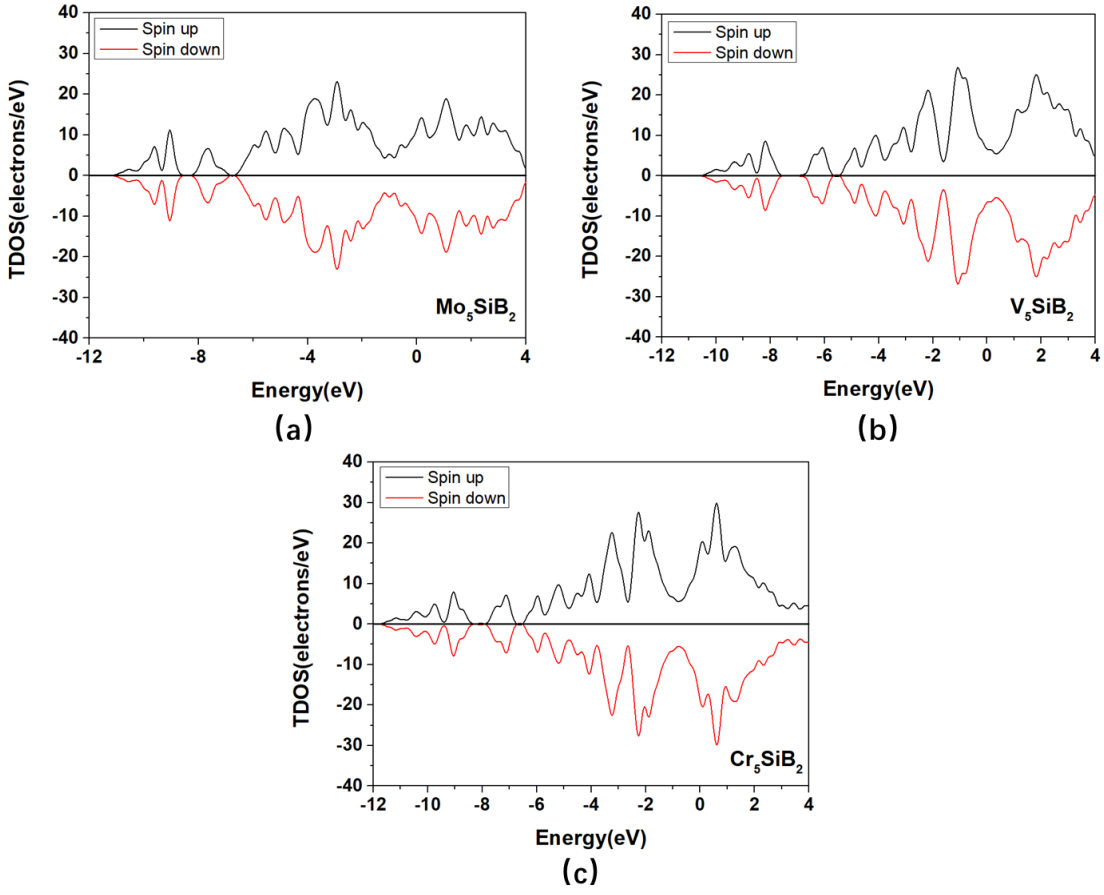

Figure S3 The spin-polarized total densities of states of Mo5SiB2 (a), V5SiB2 (b), and Cr5SiB2 (c).

Table S1 Mean bond stiffness k_{mean} in GPa of $(Zr_{0.6}Mo_{0.4})_5SiB_2$.

	B-B	M-B	M-Si	k_{min}/k_{max}
k_{mean}	1194	695	535	0.45

Table S2 Bond stiffness *k* in GPa of $(Zr_{0.6}Mo_{0.4})_5SiB_2$.

Bond	Bond stiffness	Bond	Bond stiffness	Bond	Bond stiffness
B1-B2	730	B1-Zr4	826	Si1-Zr7	625
B3-B4	1477	B1-Zr2	704	Si1-Mo3	568
B5-B6	1726	B2-Zr5	714	Si1-Mo7	490
B7-B8	490	B2-Zr6	645	Si1-Zr5	585
B1-Mo6	1014	B2-Zr3	746	Si1-Mo8	575
B1-Mo5	735	B2-Zr2	637	Si1-Zr9	588
B1-Mo3	610	B3-Zr3	658	Si1-Mo1	680
B1-Mo1	513	B3-Zr4	926	Si1-Mo2	532
B2-Mo5	813	B3-Zr2	595	Si2-Mo6	483
B2-Mo6	926	B3-Zr5	541	Si2-Zr3	599
B2-Mo4	800	B4-Zr4	633	Si2-Zr4	541
B2-Mo1	599	B4-Zr3	709	Si2-Zr8	524
B3-Mo4	758	B4-Zr2	602	Si2-Zr6	535
B3-Mo3	800	B4-Zr6	676	Si2-Zr11	444
B3-Mo6	775	B5-Zr12	585	Si2-Zr12	490
B3-Mo1	515	B5-Zr11	645	Si2-Zr10	426
B4-Mo3	794	B5-Zr7	559	Si3-Zr4	546
B4-Mo4	752	B5-Zr10	641	Si3-Zr3	526
B4-Mo5	667	B5-Zr1	735	Si3-Mo6	433
B4-Mo1	529	B6-Zr11	671	Si3-Zr8	457
B5-Mo7	775	B6-Zr12	714	Si3-Zr12	410
B5-Mo8	787	B6-Zr9	613	Si3-Zr11	463
B5-Mo2	518	B6-Zr1	625	Si3-Zr6	508
B6-Mo8	699	B6-Zr8	725	Si3-Zr10	388
B6-Mo7	741	B7-Zr9	645	Si4-Mo5	474
B6-Mo2	503	B7-Zr8	538	Si4-Mo3	575

B7-Mo7	917	B7-Zr7	546	Si4-Zr7	532
B7-Mo2	610	B7-Zr12	926	Si4-Mo8	450
B8-Mo8	685	B7-Zr1	741	Si4-Mo4	442
B8-Mo2	645	B7-Zr10	599	Si4-Zr5	510
B1-Zr5	704	B8-Zr7	565	Si4-Mo7	500
B1-Zr6	699	B8-Zr10	826	Si4-Zr9	469
/	/	Si1-Mo5	667	Si4-Zr2	741
/	/	Si1-Mo4	781	Si4-Zr1	719

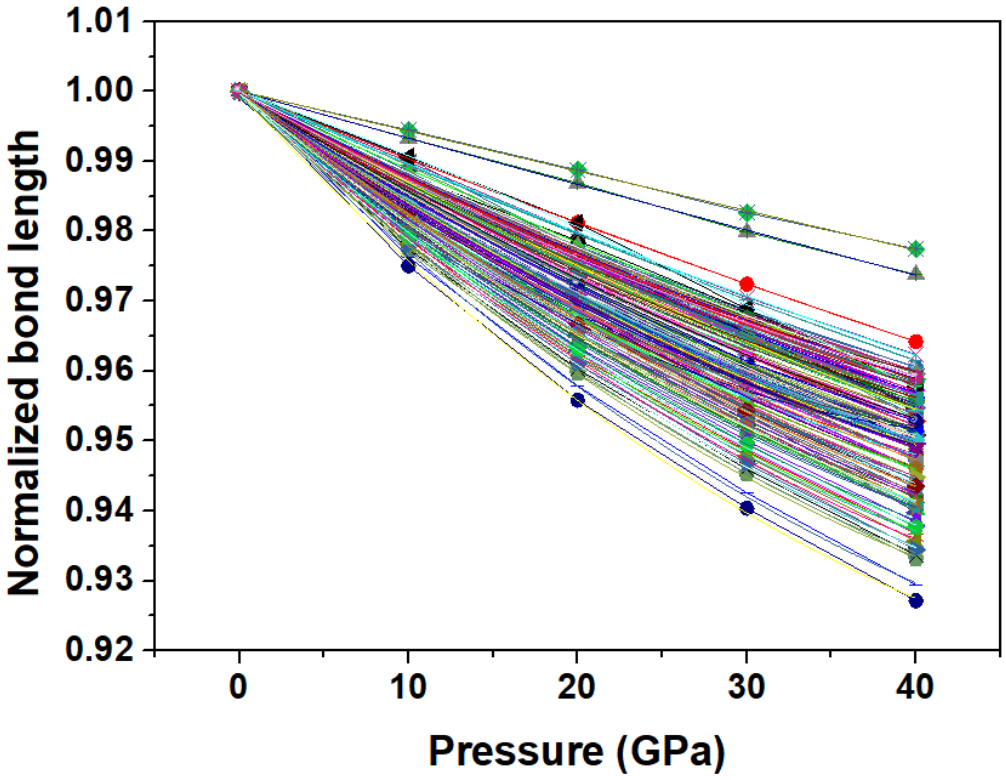

Figure S4 Normalized bond length of different types of bonds as a function of pressure in $(Zr_{0.6}Mo_{0.4})_5SiB_2$ calculated with the bond stiffness model.