Supporting Information

Pressure tuned structural, electronic and elastic properties of $U_3Si_2C_2$: a first principles study

Table S1 The lattice parameters of the optimized cells. The positions of atoms along c axis (0, 0, z) are listed.

Pressure (GPa)	a=b (Å)	c(Å)	z(U1) (Å)	z(U2) (Å)	z(Si) (Å)	z(C) (Å)
0	3.651	18.052	0	3.249	7.465	5.543
4	3.615	17.749	0	3.174	7.367	5.457
8	3.588	17.553	0	3.123	7.296	5.382
9.8	3.574	17.440	0	3.097	7.259	5.349
10	3.574	18.026	0	3.246	7.422	5.526
12	3.562	17.920	0	3.220	7.386	5.493
16	3.540	17.709	0	3.169	7.313	5.427
20	3.520	17.526	0	3.125	7.249	5.369
24	3.501	17.363	0	3.085	7.192	5.317

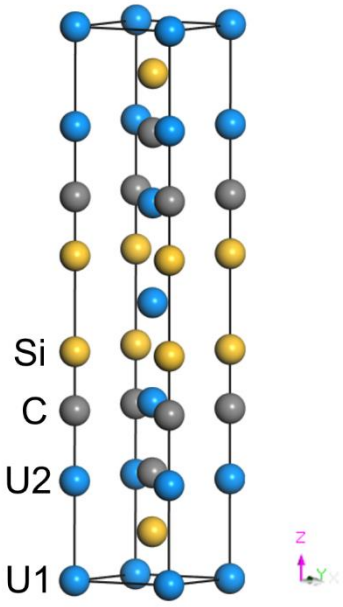

Figure S1 The crystal structure of $U_3Si_2C_2$ (blue: uranium; grey: carbon; yellow: silicon). The atoms listed in Table S1 have been marked.

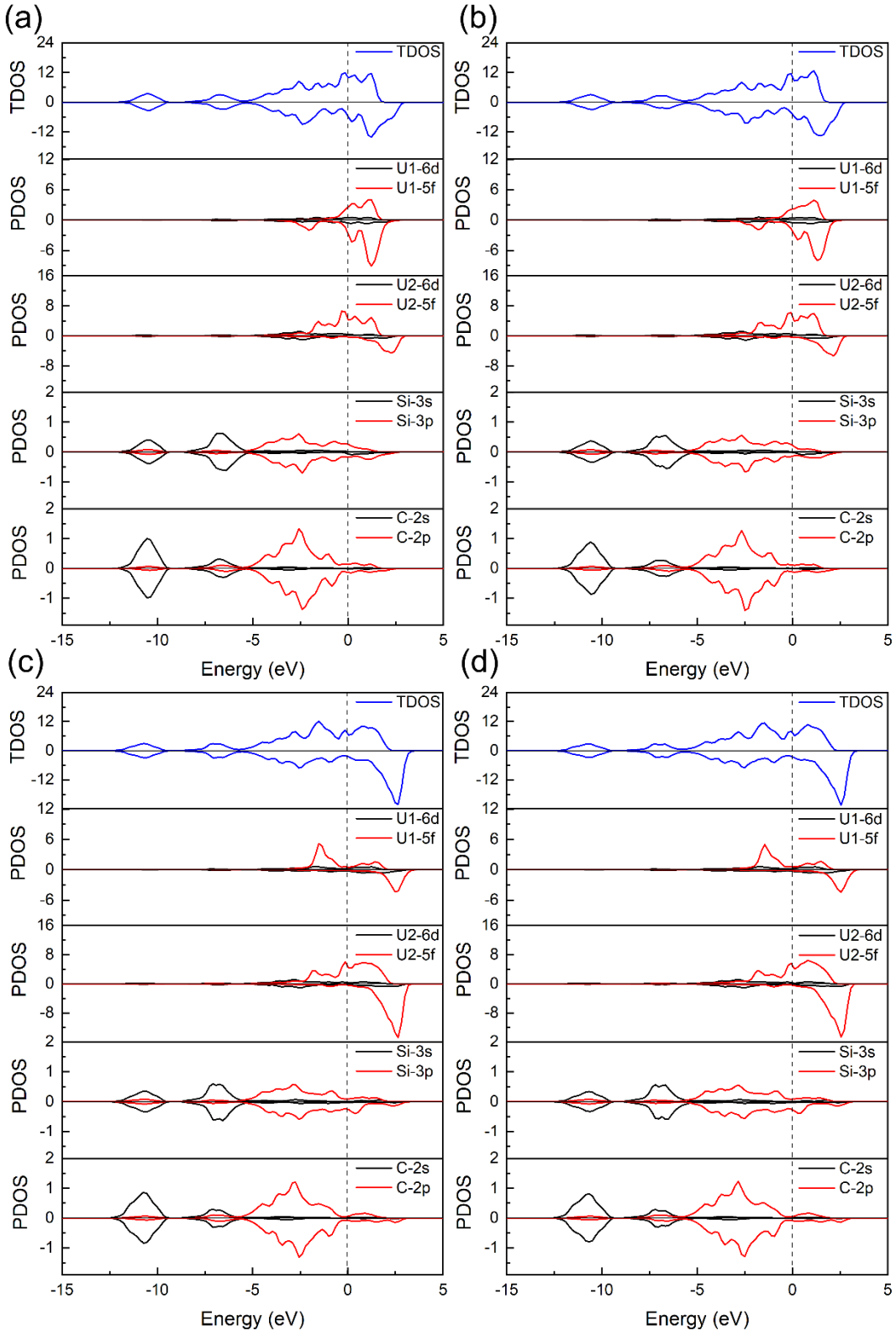

Figure S2 The total density of state (TDOS) and partial density of state (PDOS) of $U_3Si_2C_2$ under different pressures: (a) 0 GPa; (b) 8GPa; (c) 12GPa and (d) 16GPa. The dash line represents Fermi energy.