Parameter	TaAs	TaP	NbAs	NbP
a (Å)	3.466 (3.437)	3.339 (3.318)	3.477 (3.452)	3.350 (3.334)
c (Å)	11.750 (11.656)	11.486 (11.363)	11.752 (11.679)	11.424 (11.376)
u	0.417 (0.417)	0.414 (0.416)	0.422 (0.417)	0.416 (0.416)
B (GPa)	84.38	102.31	87.47	95.99
B'	4.14	4.05	4.05	3.85
E_{coh} (eV/pair)	14.27	16.00	15.09	16.69

Table 1. Calculated lattice parameters a, c, and u of transition metal monopnictides. Experimental values (adapted from collection in[26]) are given in parenthesis. In addition, elastic and energetic parameters, the bulk modulus B, its pressure derivative B', and the cohesive energy E_{coh}, are listed.

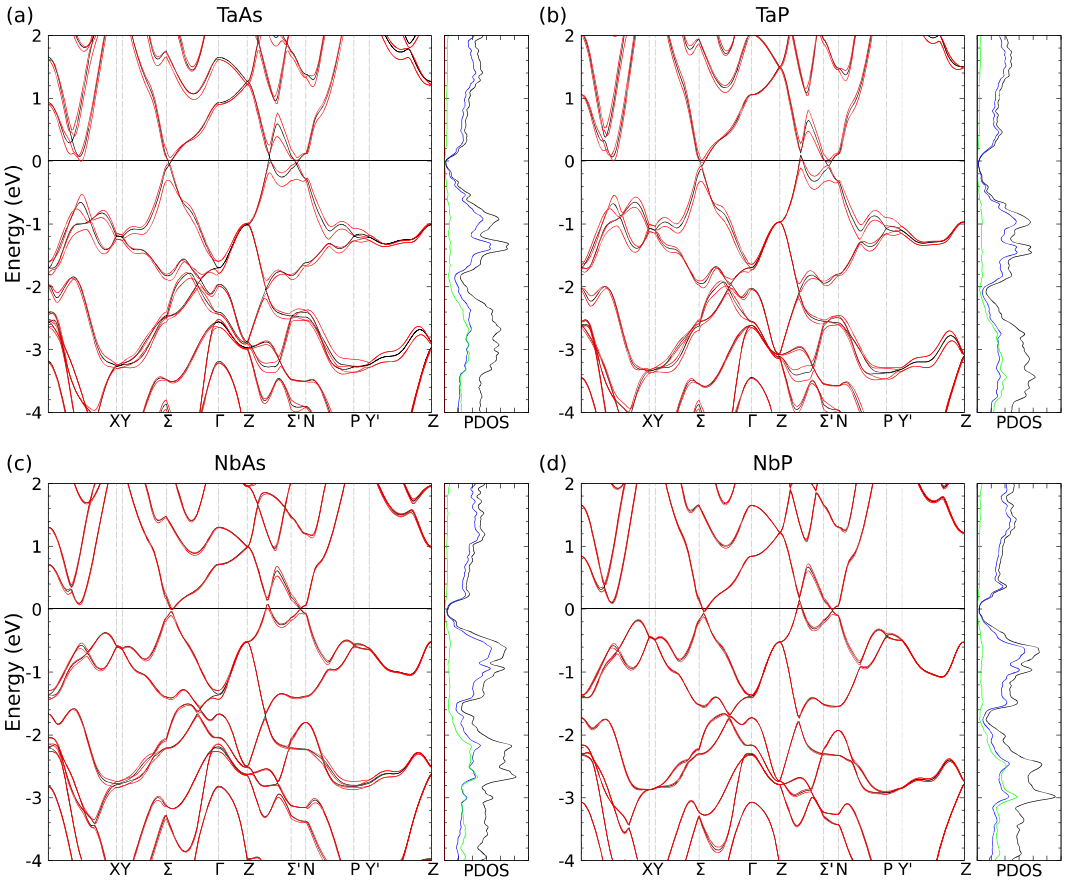

Figure 2. Band structure with SOI (red solid lines) and without SOI (black solid lines) of (**a**) TaAs, (**b**) TaP, (**c**) NbAs, and (**d**) NbP along high-symmetry lines in the bct BZ in Fig. 1b. The Fermi energy ε_F (black horizontal line) is chosen as energy zero. In addition, the DOS (black lines) and the orbital-symmetry-resolved DOS (Ta6*s* and Nb5*s*: red lines, Ta5*d* and Nb4*d*: blue lines, and As4*p* and P3*p*: green lines) are plotted.

definition of Wyckhoff positions. The internal cell parameters u agree well with measured values and with the rule $u \sim 5/12$ found experimentally[30]. The calculated a and c lattice constants slightly overestimate the experimental ones by 0.4–0.8%. Only in the case of the c lattice constant of TaP the deviation is slightly larger with 1.1%. The reason for the general overestimation is the used PBE XC functional with gradient corrections[34]. There are also other experimental values $a = 3.4348$ Å and $c = 11.641$ Å for TaAs[30], which are, also, close to our computed results.

Band structures. The band structures of the four transition metal monopnictides TaAs, TaP, NbAs, and NbP are plotted in Fig. 2 along several high-symmetry lines in the bct BZ (see Fig. 1b). Since the bonds are highly ionic, the cations (anions) approach +3 (−3) charged ions, suggesting completely filled p^6 shells of the anions and partially filled d^2 shells of the cations, which build the upper valence bands. The orbital-resolved density of states (DOS) of the four compounds given also in Fig. 2 shows that Ta6*s* and Nb5*s* states are not visible in the presented energy range around the Fermi level.