First-principles exploration of superconductivity in MXenes

Supplementary Information

J. Bekaert,[1] C. Sevik,[2] and M. V. Milošević[1]
[1]Department of Physics & NANOlab Center of Excellence, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium
[2]Department of Mechanical Engineering, Faculty of Engineering, Eskisehir Technical University, 26555 Eskisehir, Turkey

FERMI SURFACES

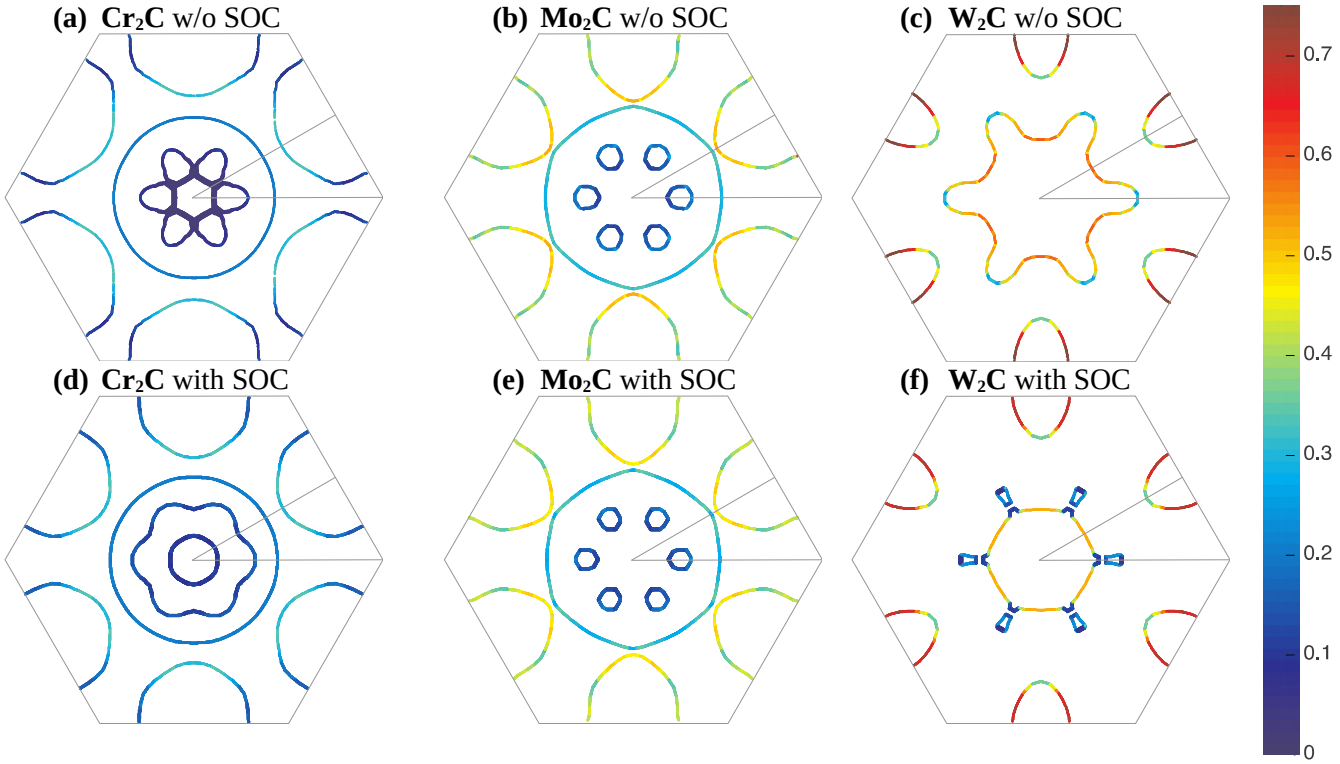

Figure 1: Calculated Fermi surfaces. Line color shows the calculated Fermi velocity in 10^6 ms^{-1}.

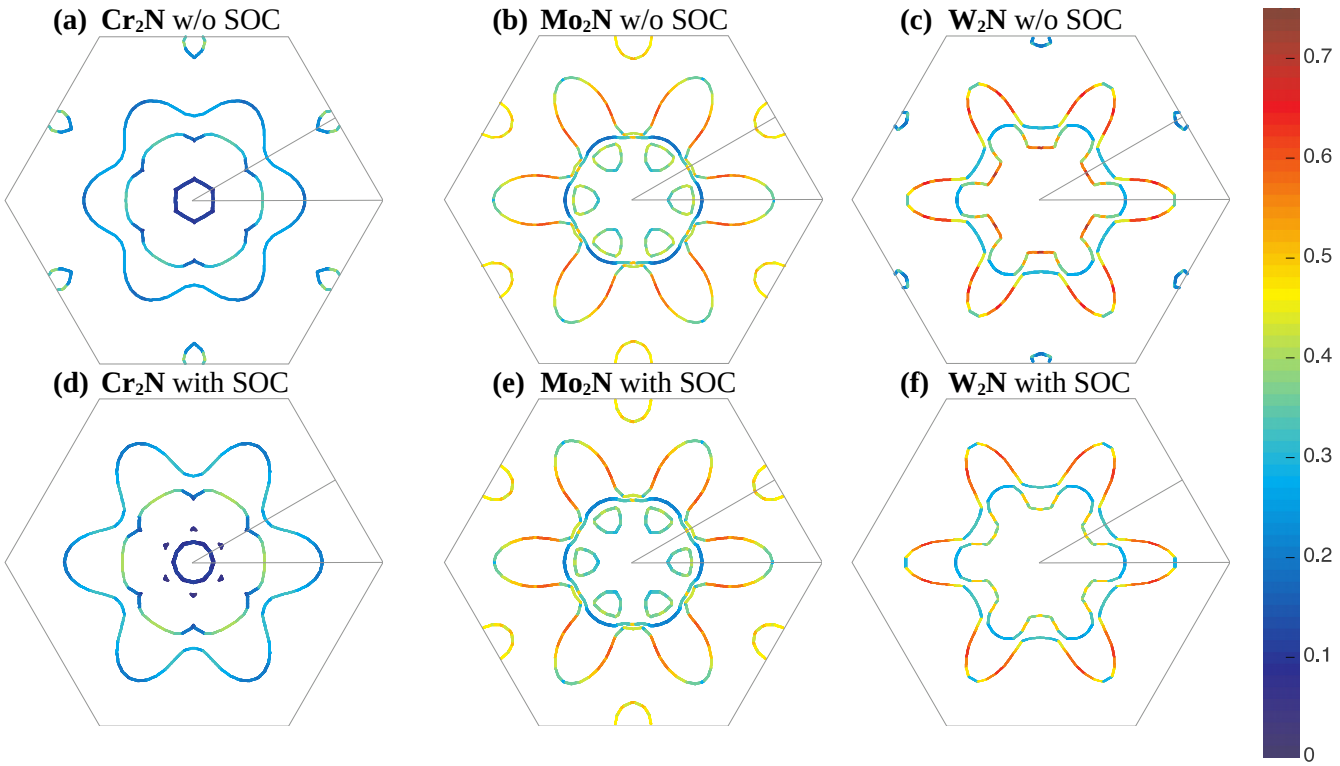

Figure 2: Calculated Fermi surfaces. Line color shows the calculated Fermi velocity in 10^6 ms^{-1}.

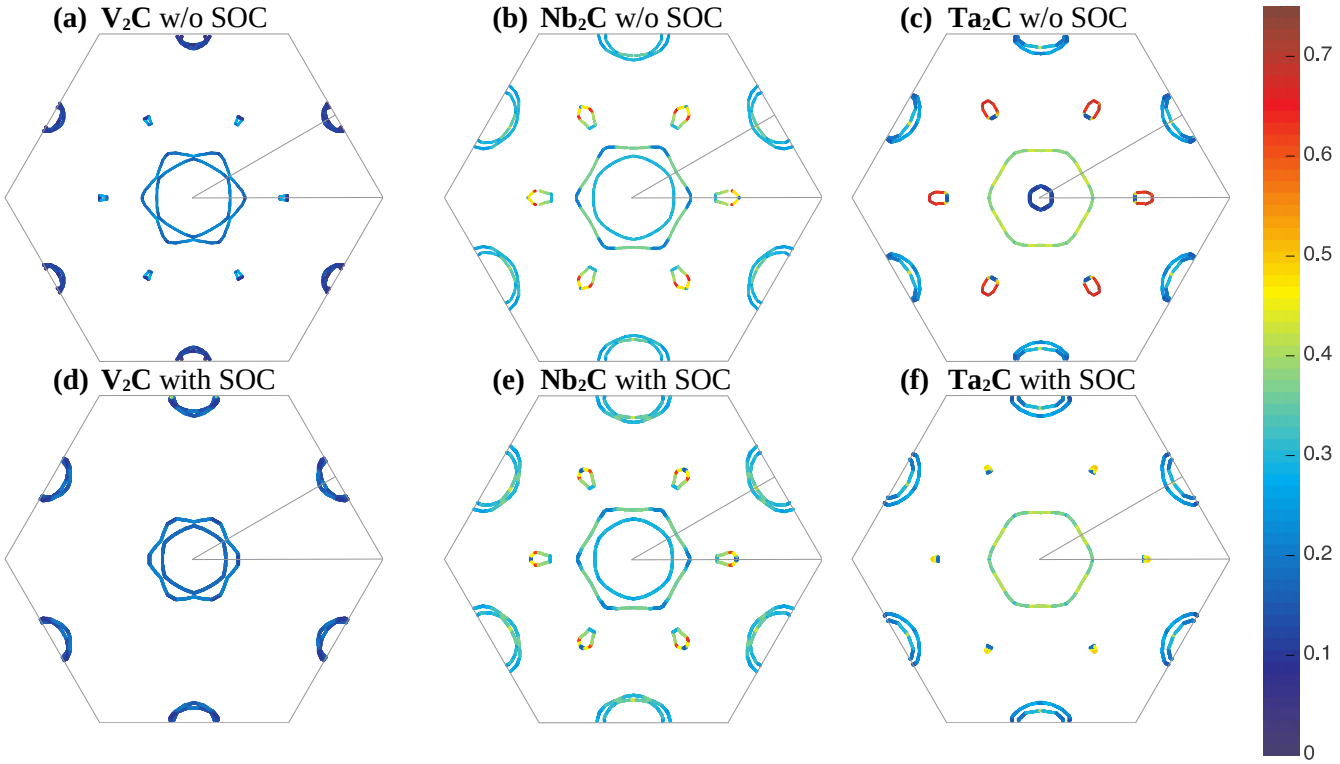

Figure 3: Calculated Fermi surfaces. Line color shows the calculated Fermi velocity in 10^6 ms^{-1}.

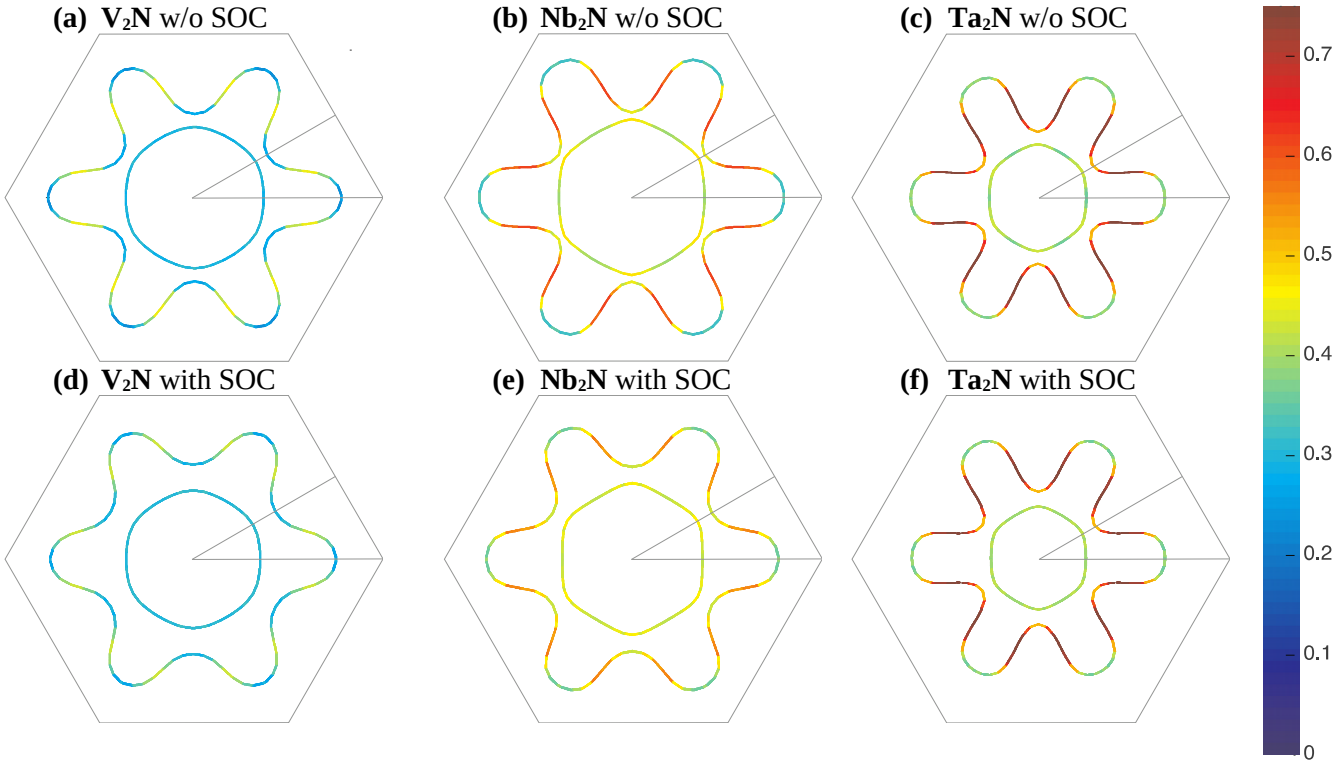

Figure 4: Calculated Fermi surfaces. Line color shows the calculated Fermi velocity in 10^6 ms^{-1}.

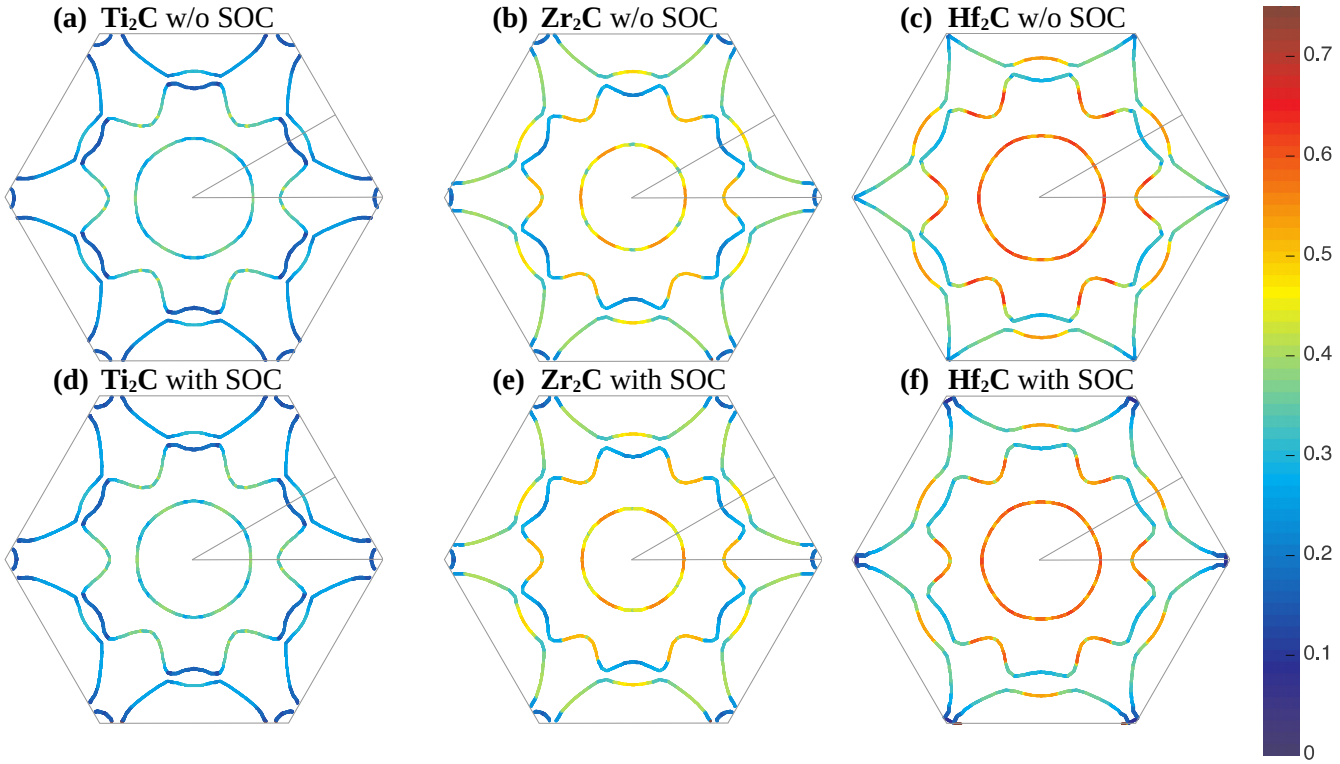

Figure 5: Calculated Fermi surfaces. Line color shows the calculated Fermi velocity in 10^6 ms^{-1}.

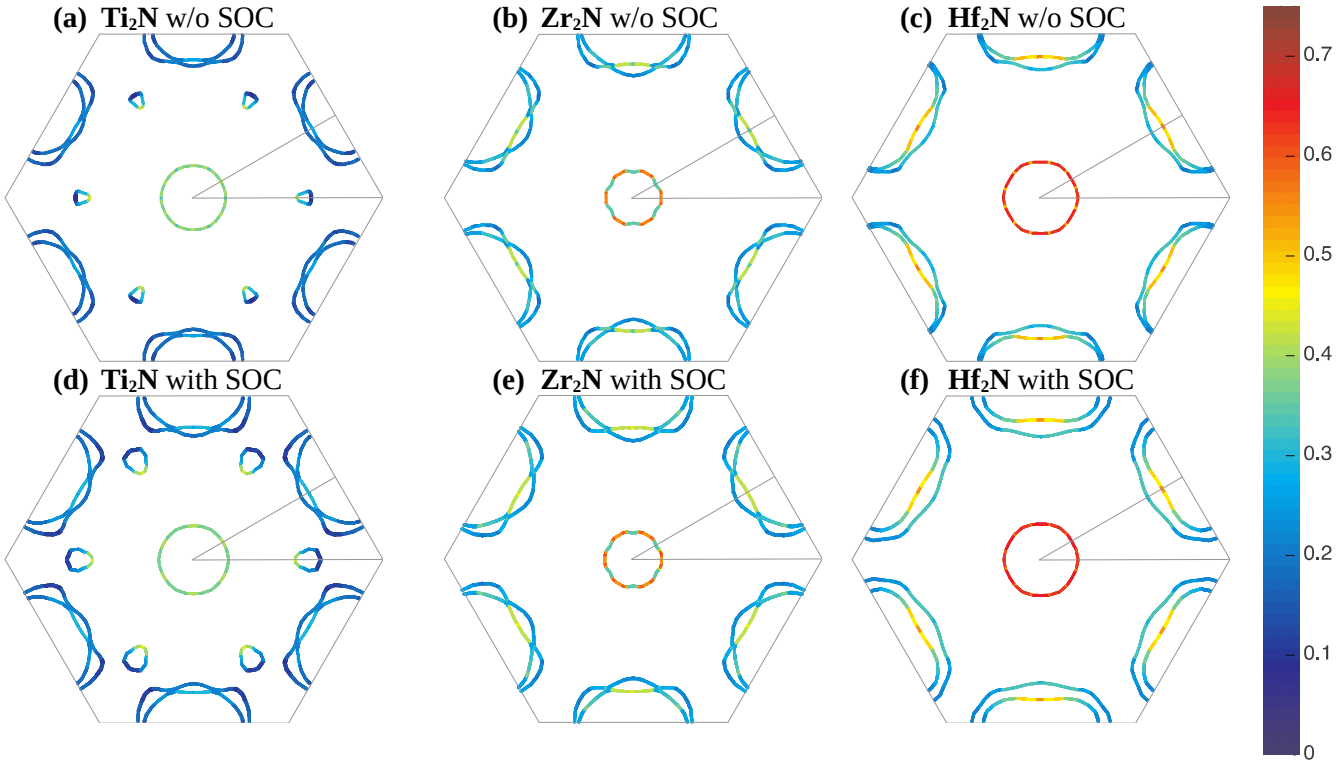

Figure 6: Calculated Fermi surfaces. Line color shows the calculated Fermi velocity in 10^6 ms^{-1}.

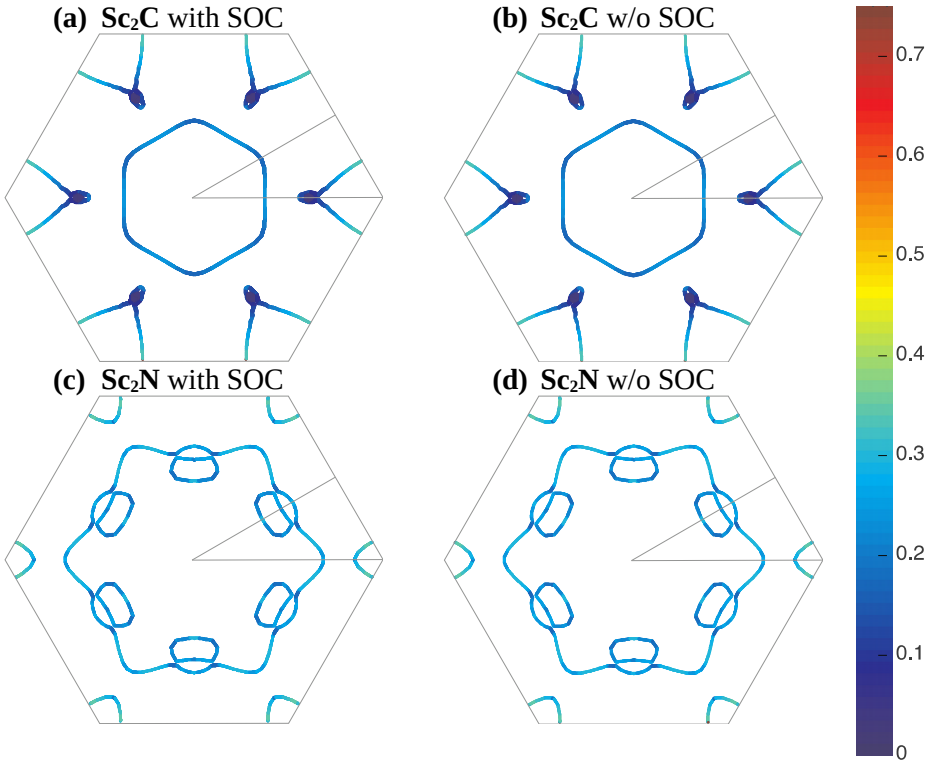

Figure 7: Calculated Fermi surfaces. Line color shows the calculated Fermi velocity in 10^6 ms^{-1}.

ELECTRON-PHONON COUPLING – CARBIDES

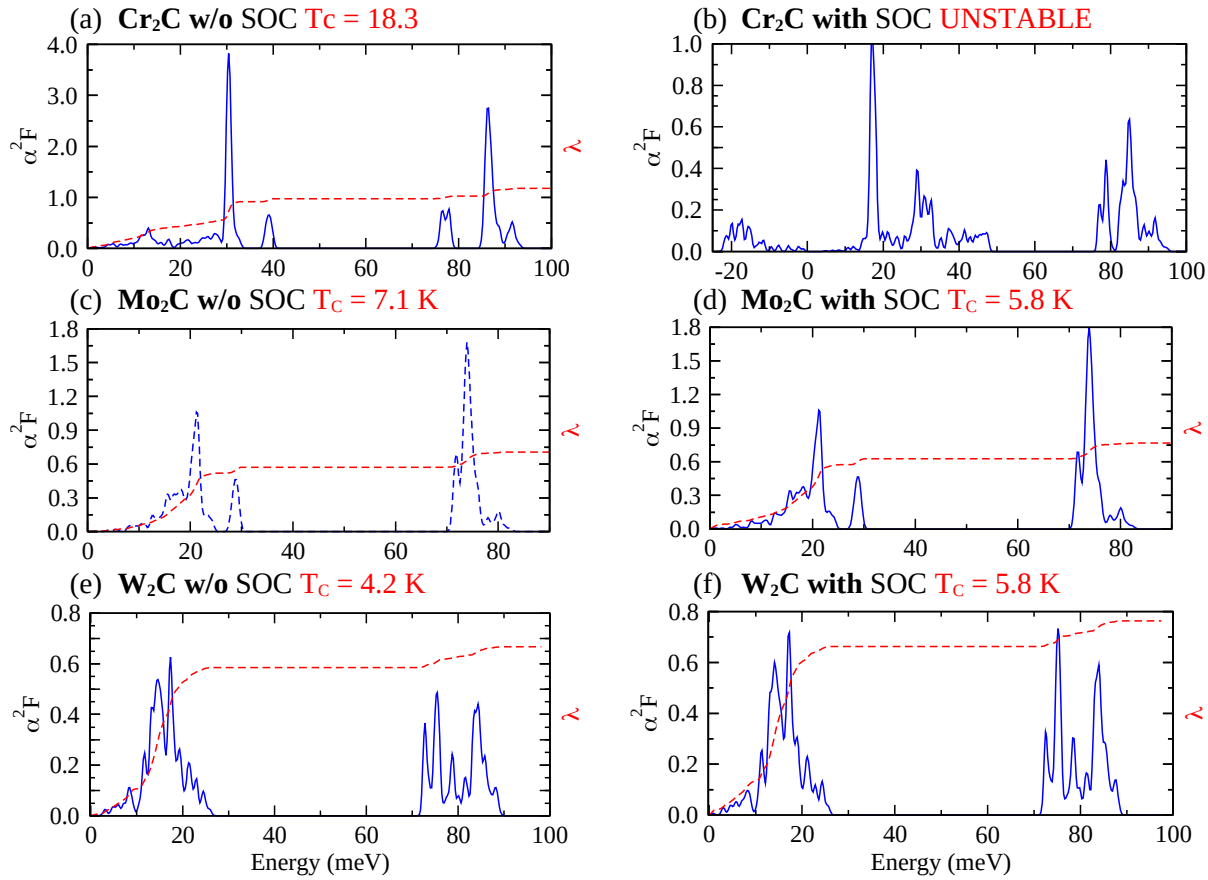

Figure 8: The isotropic Eliashberg function $\alpha^2F(\omega)$ and resulting electron-phonon coupling λ.

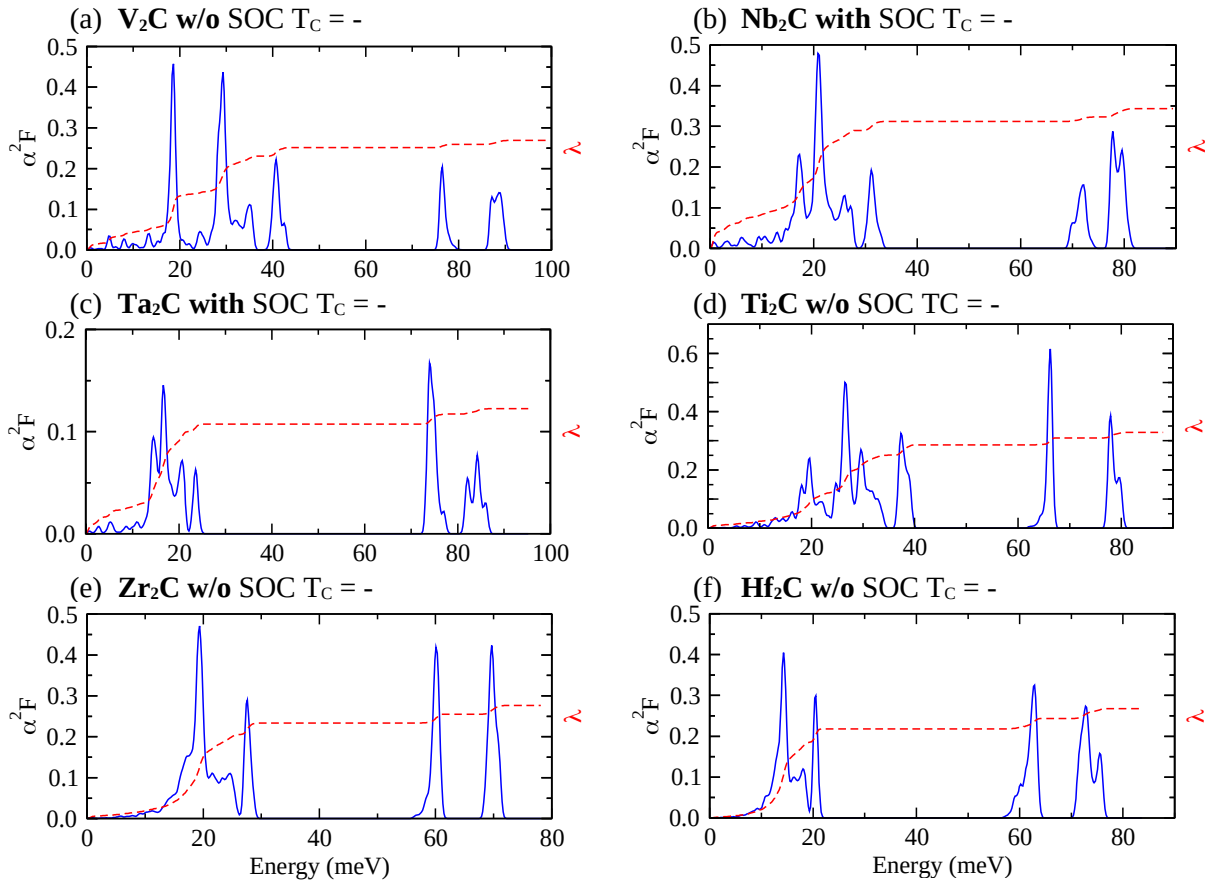

Figure 9: The isotropic Eliashberg function $\alpha^2F(\omega)$ and resulting electron-phonon coupling λ.

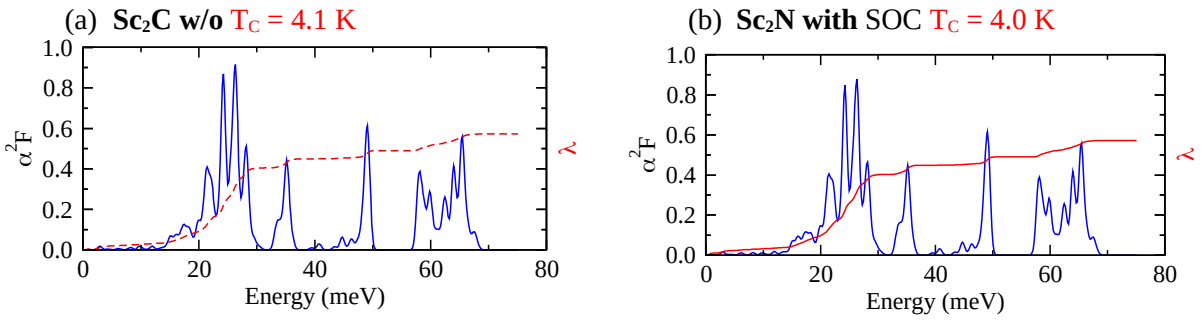

Figure 10: The isotropic Eliashberg function $\alpha^2F(\omega)$ and resulting electron-phonon coupling λ.

ELECTRON-PHONON COUPLING – NITRIDES

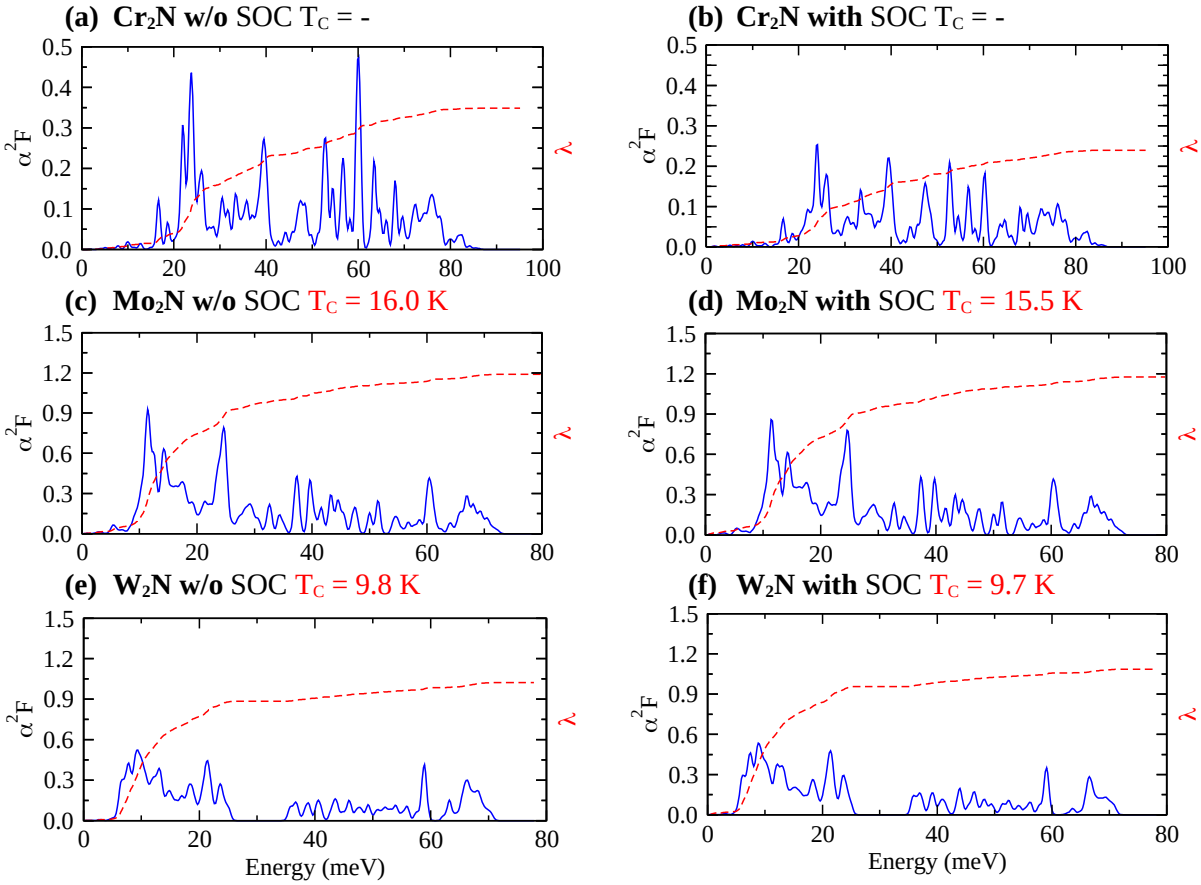

Figure 11: The isotropic Eliashberg function $\alpha^2F(\omega)$ and resulting electron-phonon coupling λ.

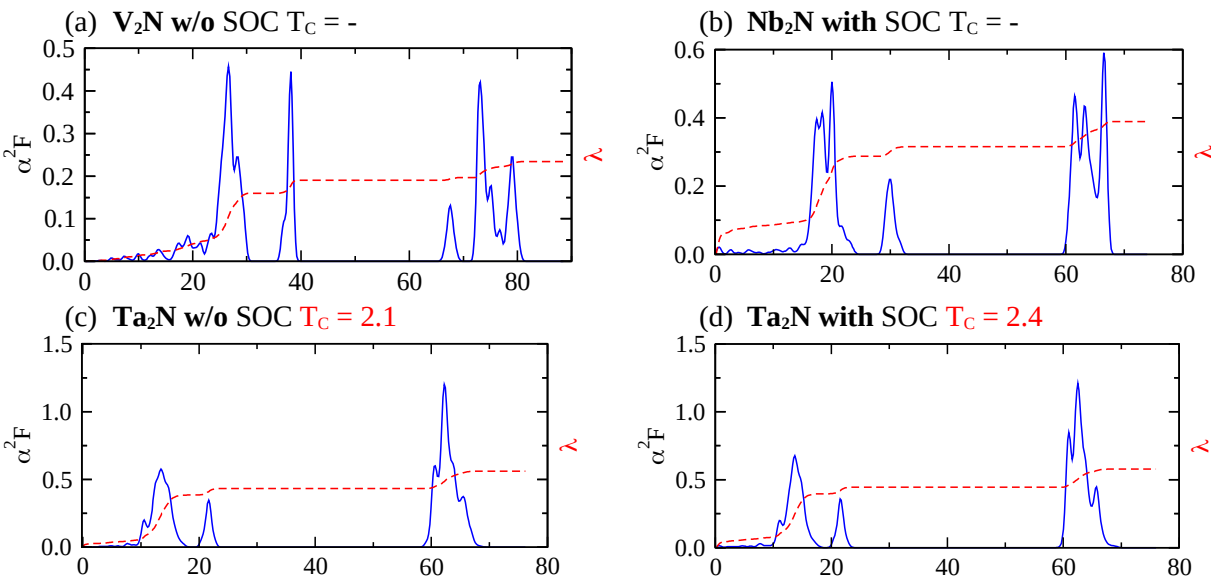

Figure 12: The isotropic Eliashberg function $\alpha^2F(\omega)$ and resulting electron-phonon coupling λ.

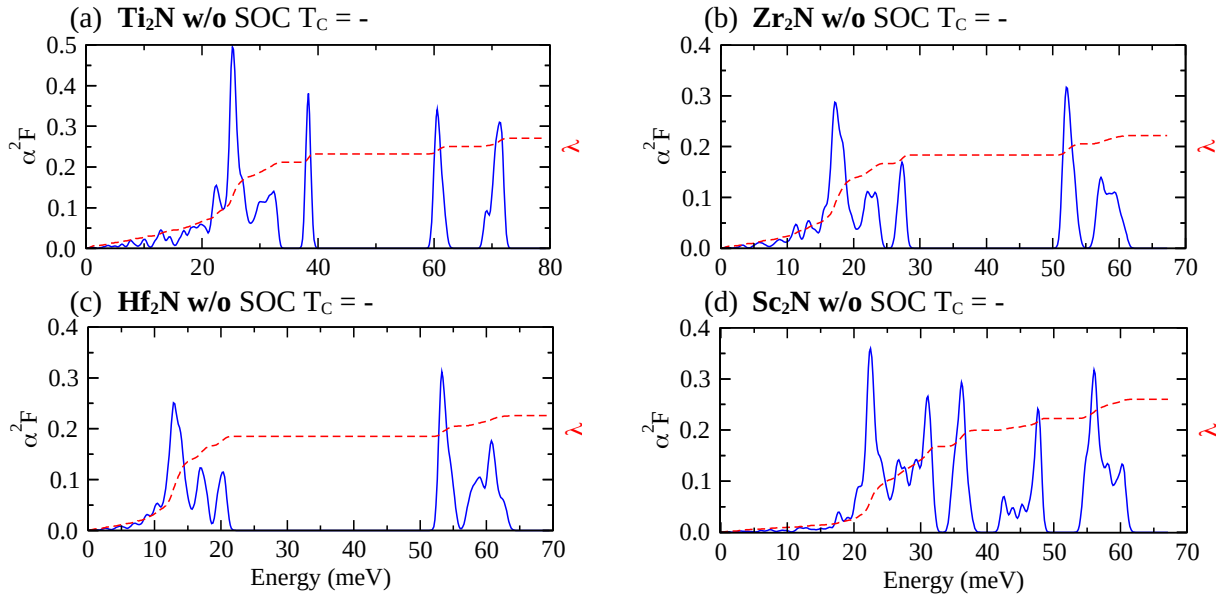

Figure 13: The isotropic Eliashberg function $\alpha^2F(\omega)$ and resulting electron-phonon coupling λ.

BAND STRUCTURES – CARBIDES

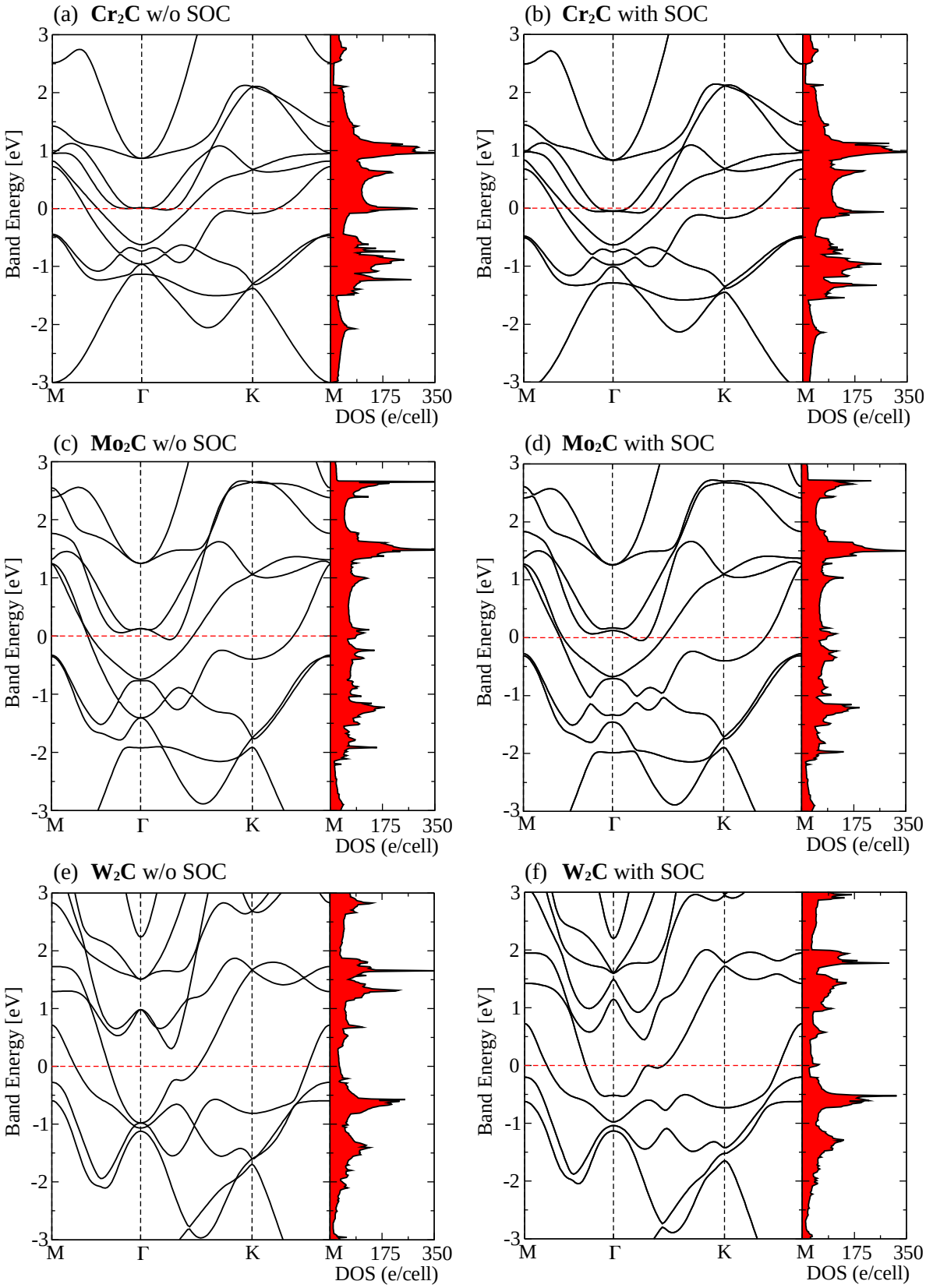

Figure 14: The band structure of M_2C (M = Cr, Mo, W) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in electrons/Hartree/cell.

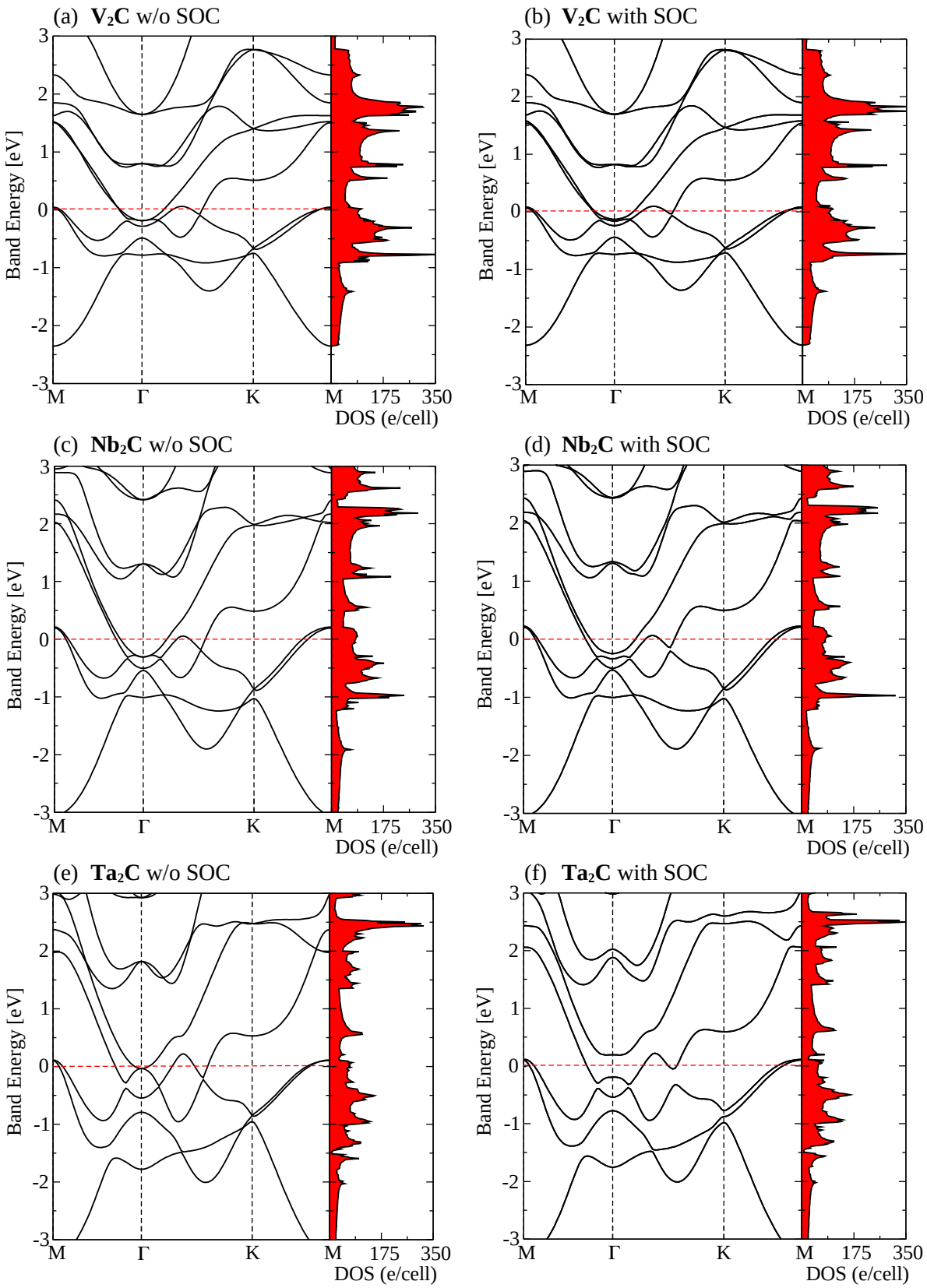

Figure 15: The band structure of M_2C (M = V, Nb, Ta) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in electrons/Hartree/cell.

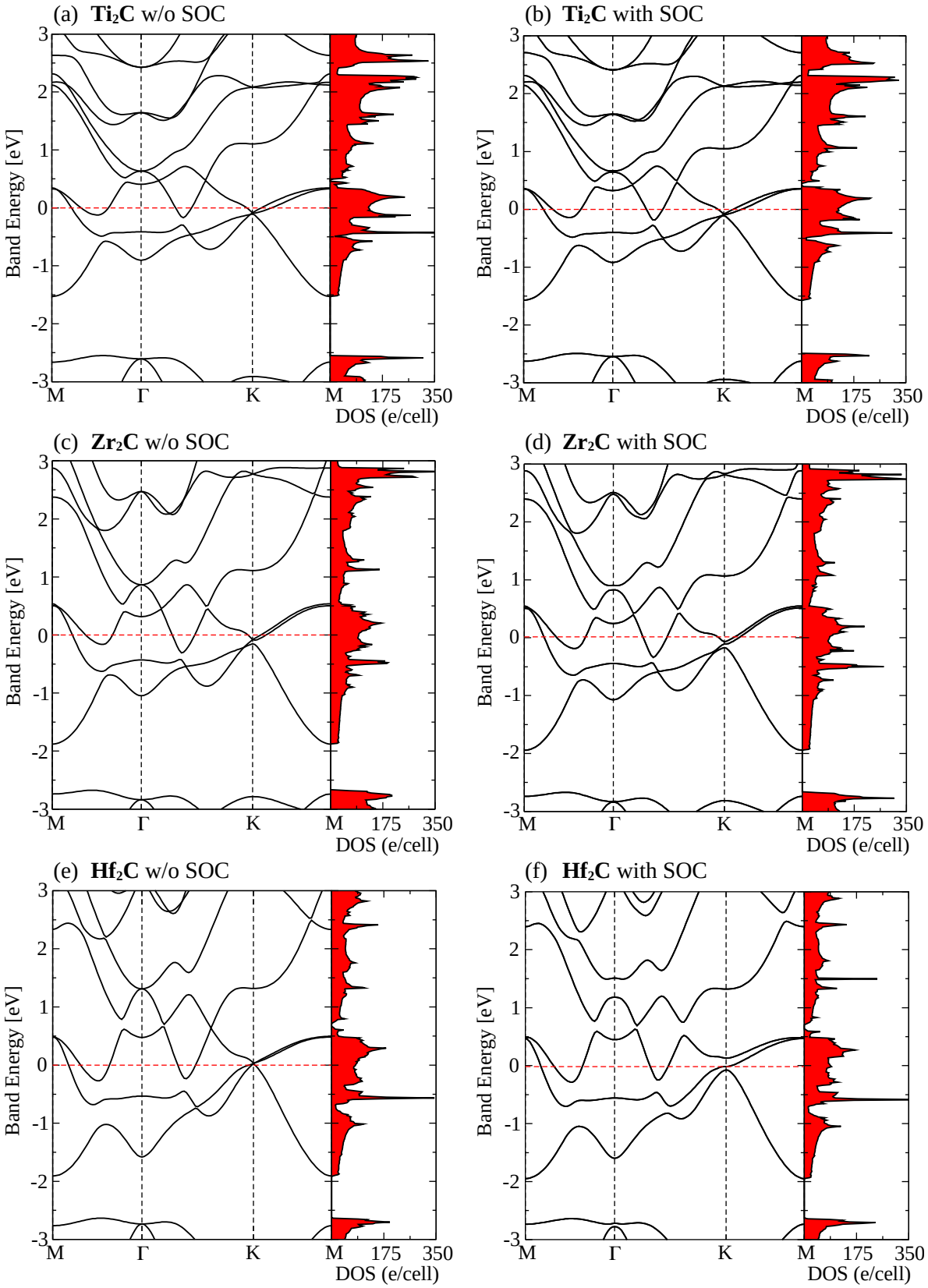

Figure 16: The band structure of M_2C (M = Ti, Zr, Hf) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in electrons/Hartree/cell.

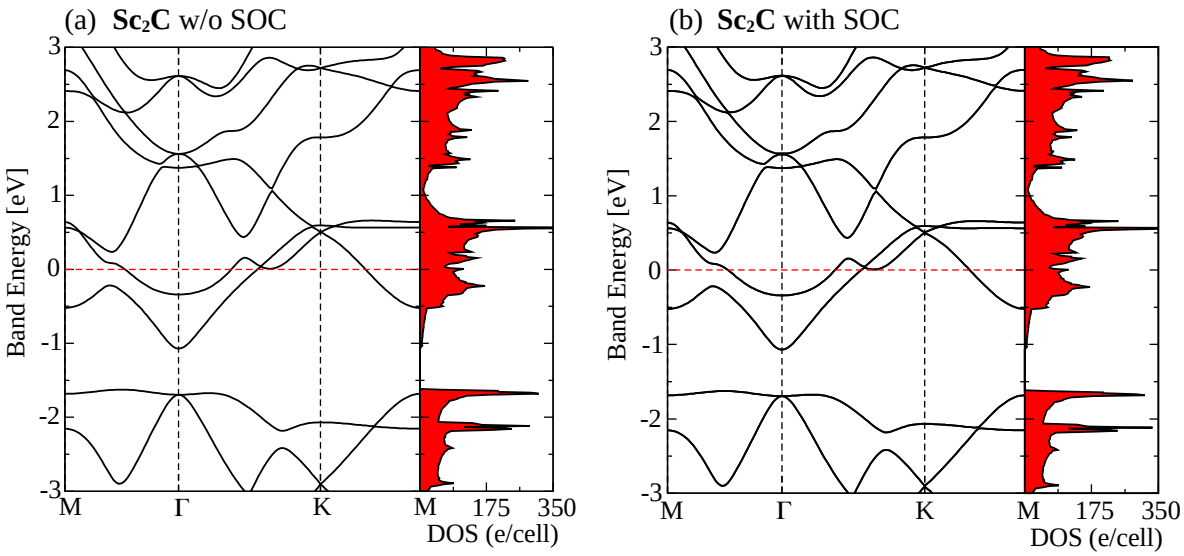

Figure 17: The band structure of Sc_2C with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in electrons/Hartree/cell.

BAND STRUCTURES – NITRIDES

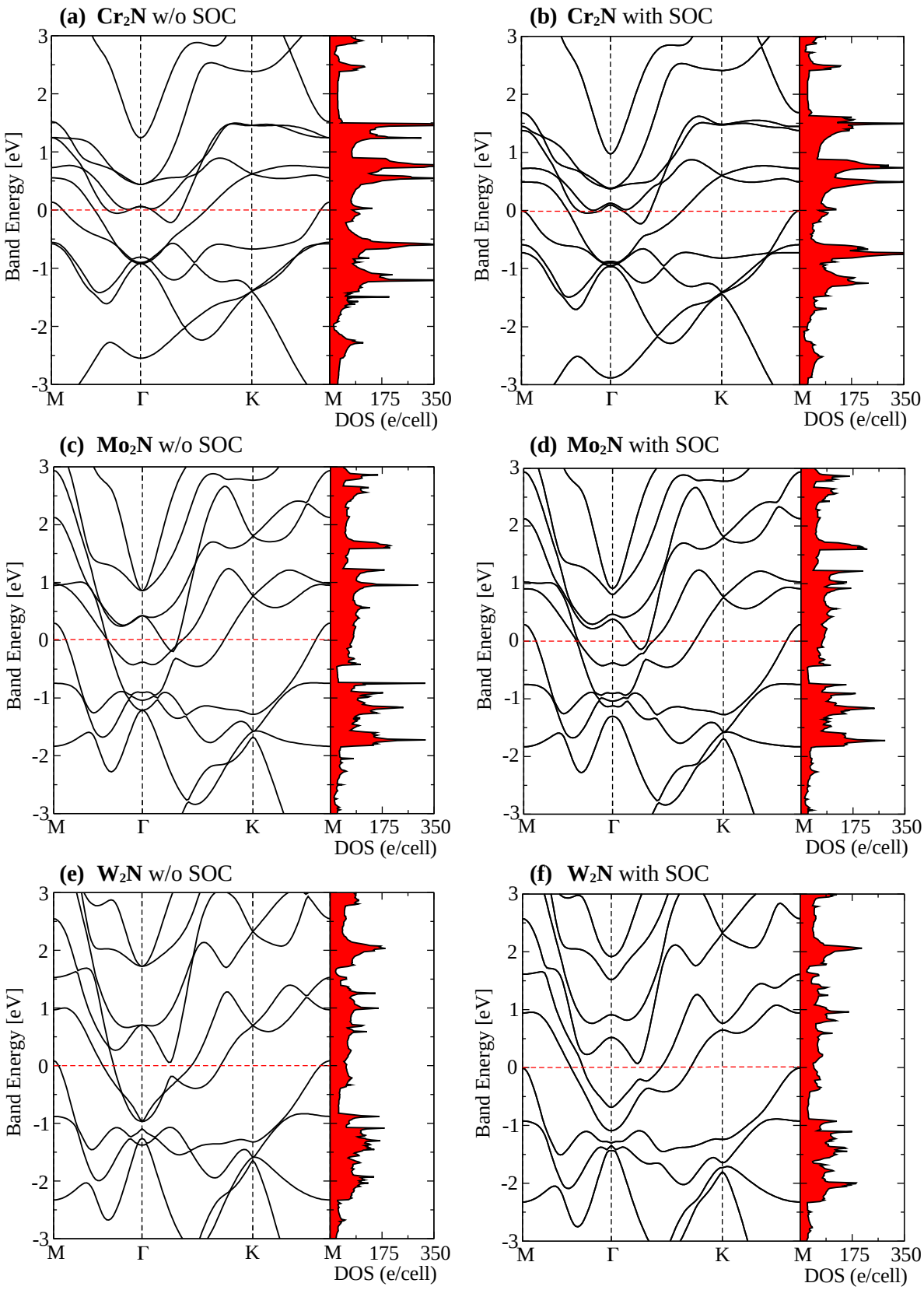

Figure 18: The band structure of M_2N (M = Cr, Mo, W) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in electrons/Hartree/cell.

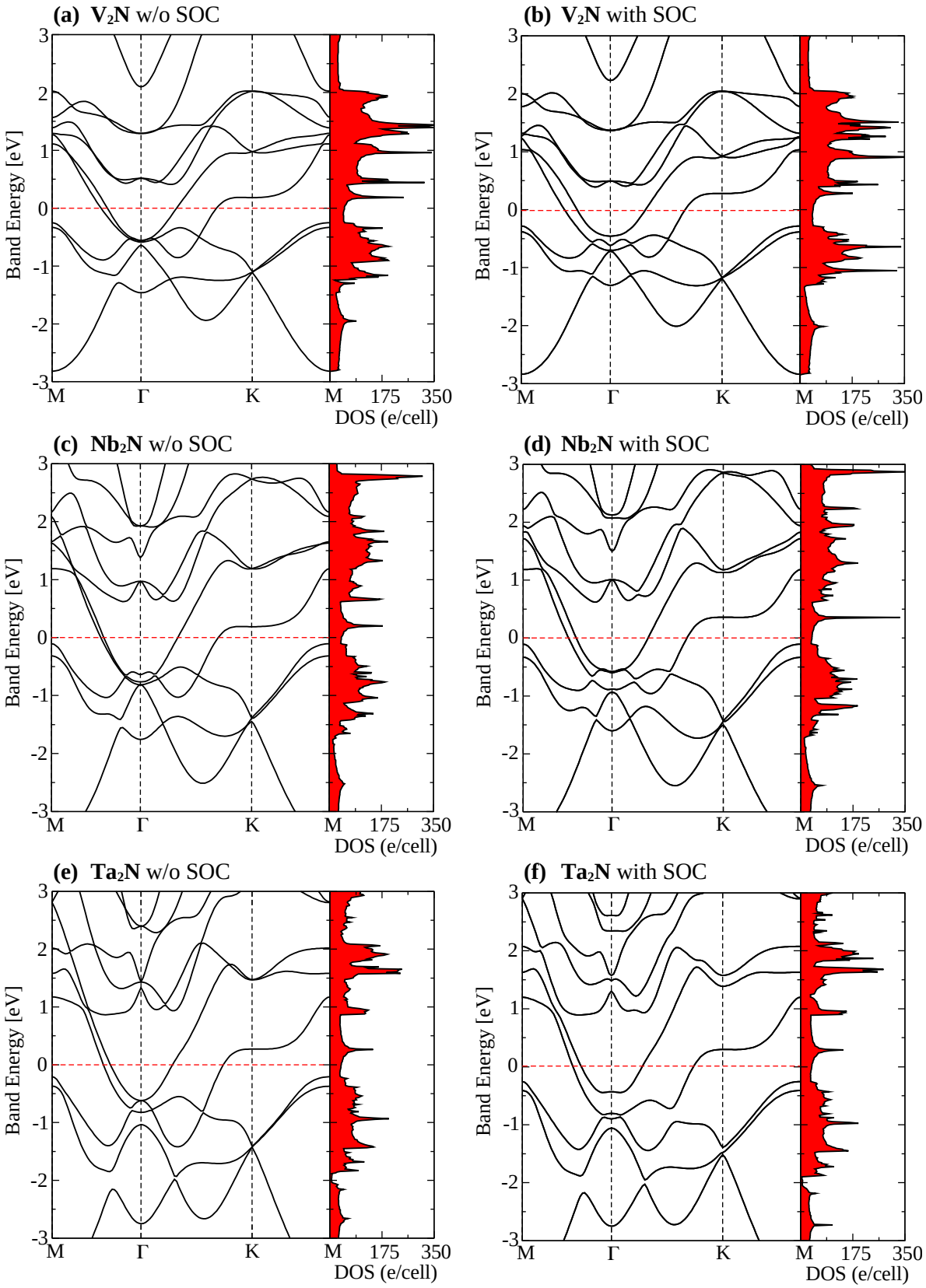

Figure 19: The band structure of M_2N (M = V, Nb, Ta) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in electrons/Hartree/cell.

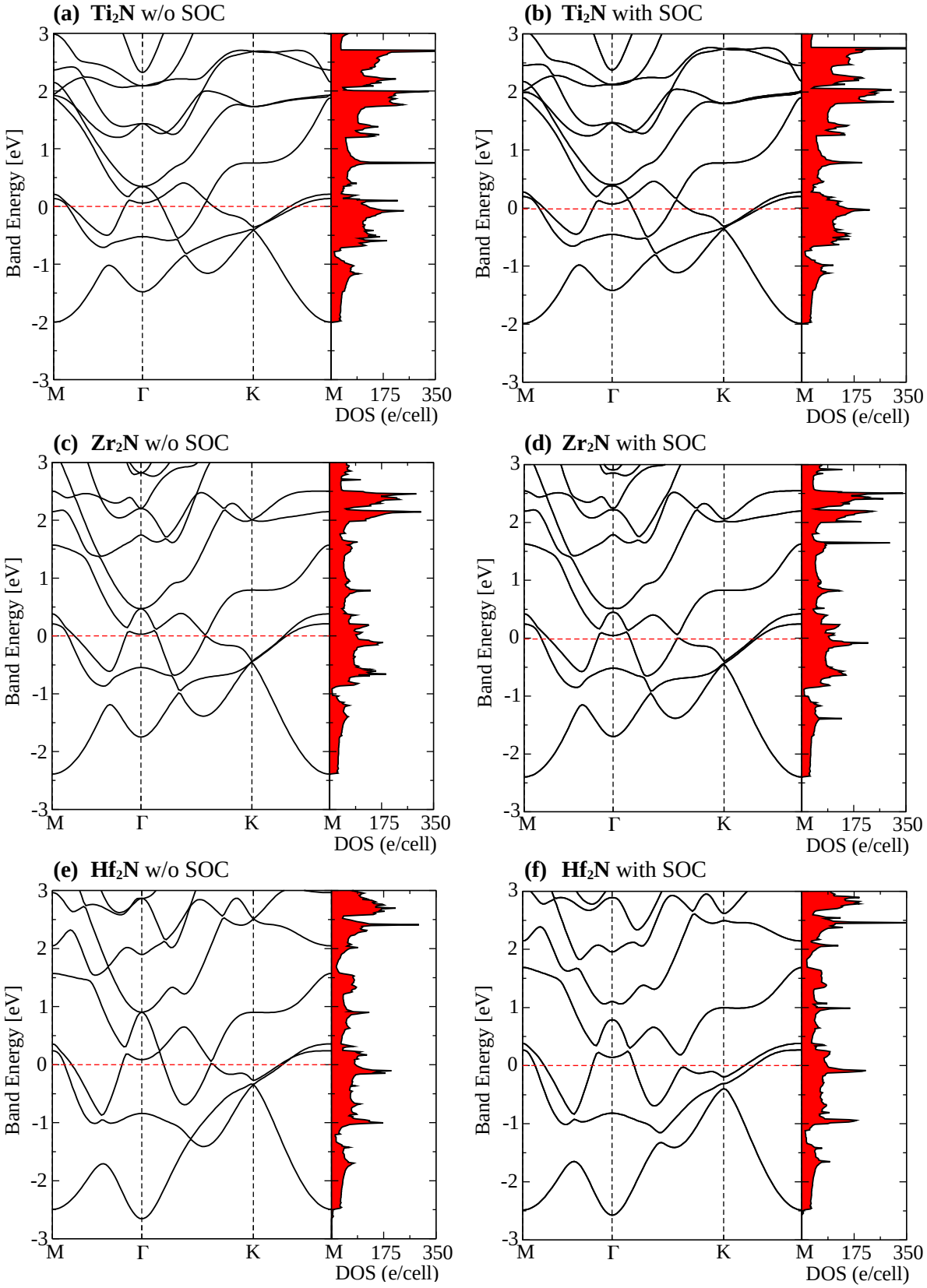

Figure 20: The band structure of M_2N (M = Ti, Zr, Hf) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in electrons/Hartree/cell.

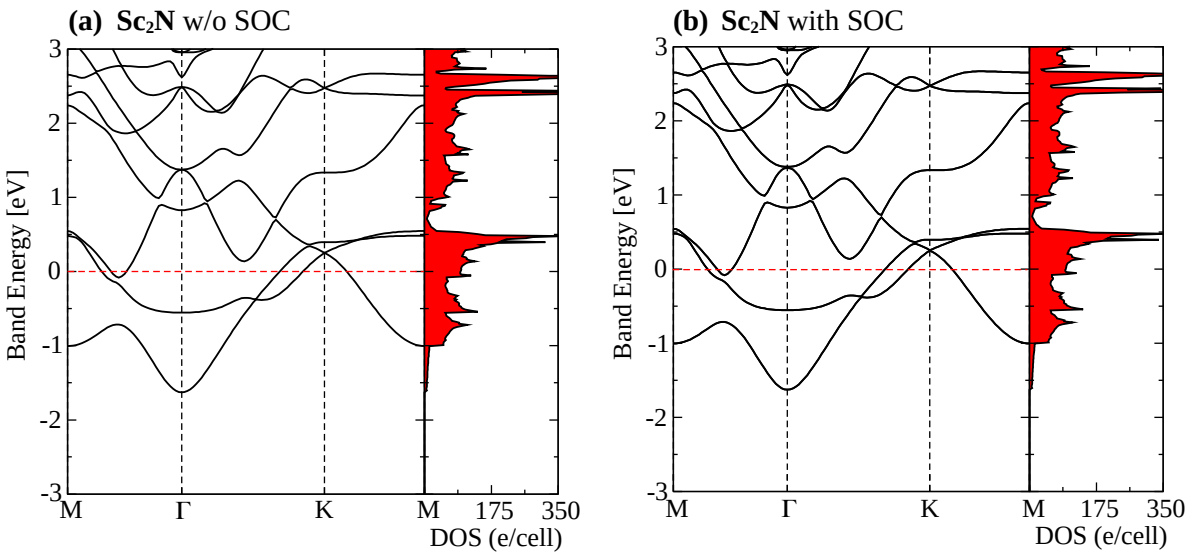

Figure 21: The band structure of Sc_2N with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in electrons/Hartree/cell.

PHONON SPECTRUM – CARBIDES

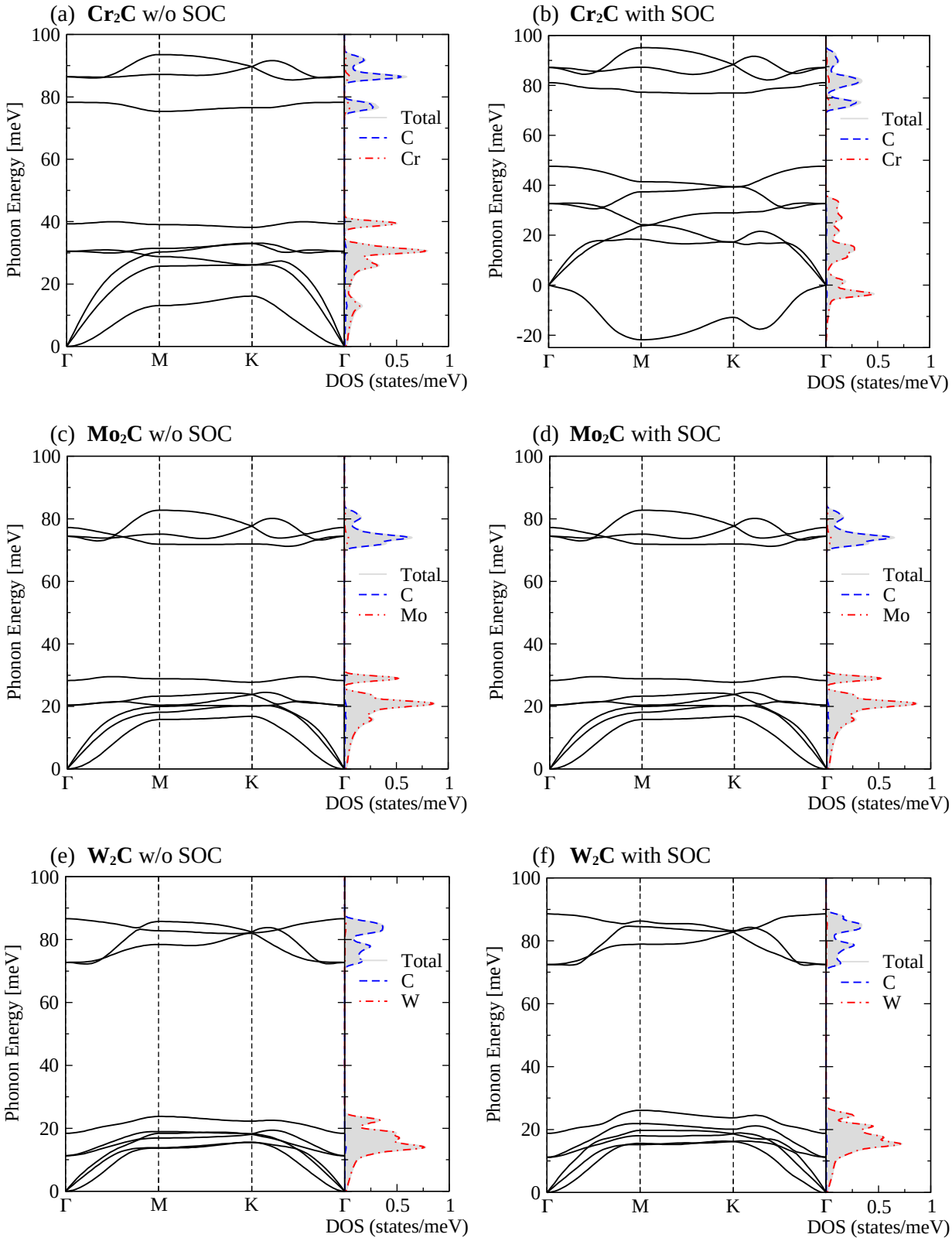

Figure 22: Vibrational spectrum of M_2C (M = Cr, Mo, W) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in states/meV.

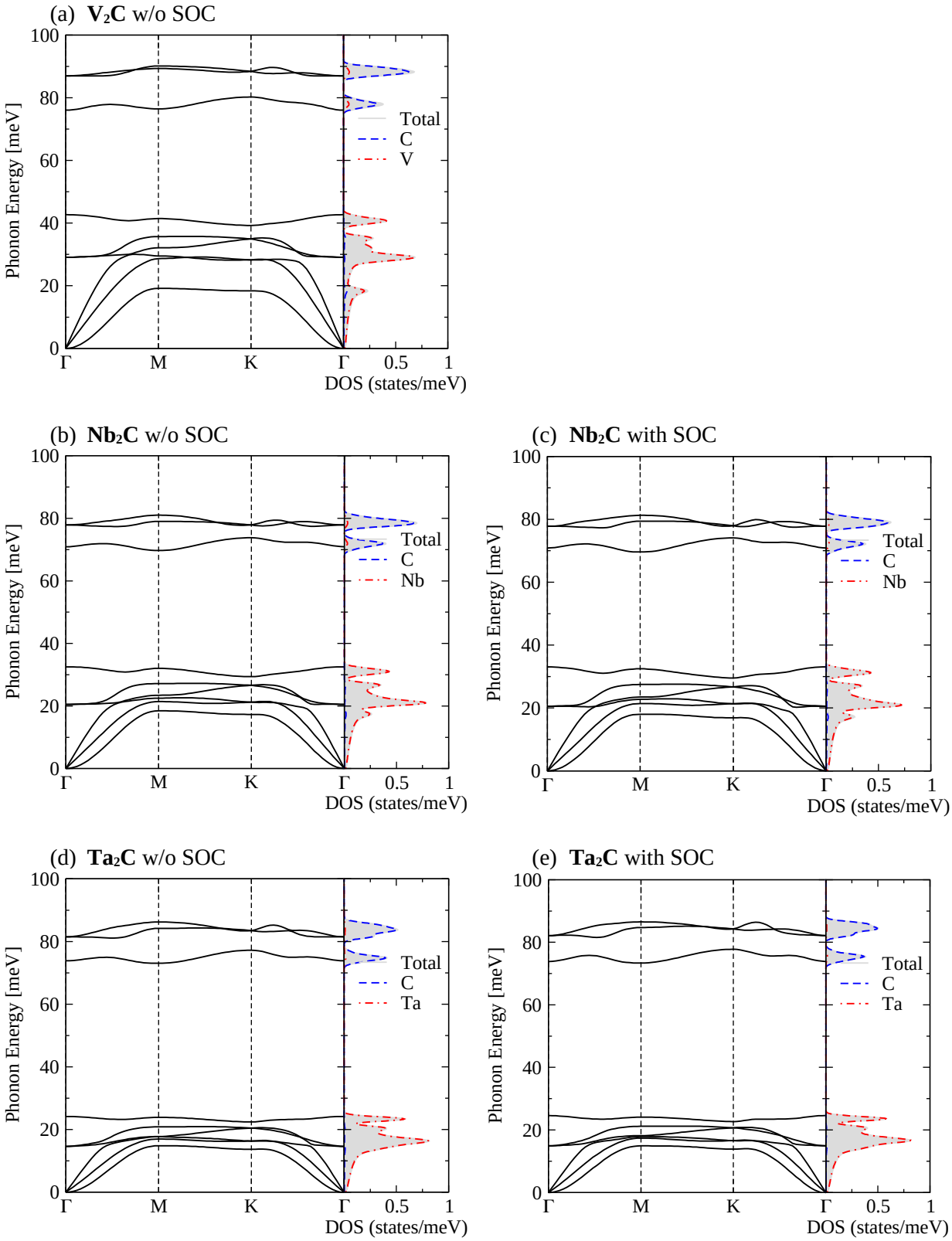

Figure 23: Vibrational spectrum of M_2C (M = V, Nb, Ta) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in states/meV.

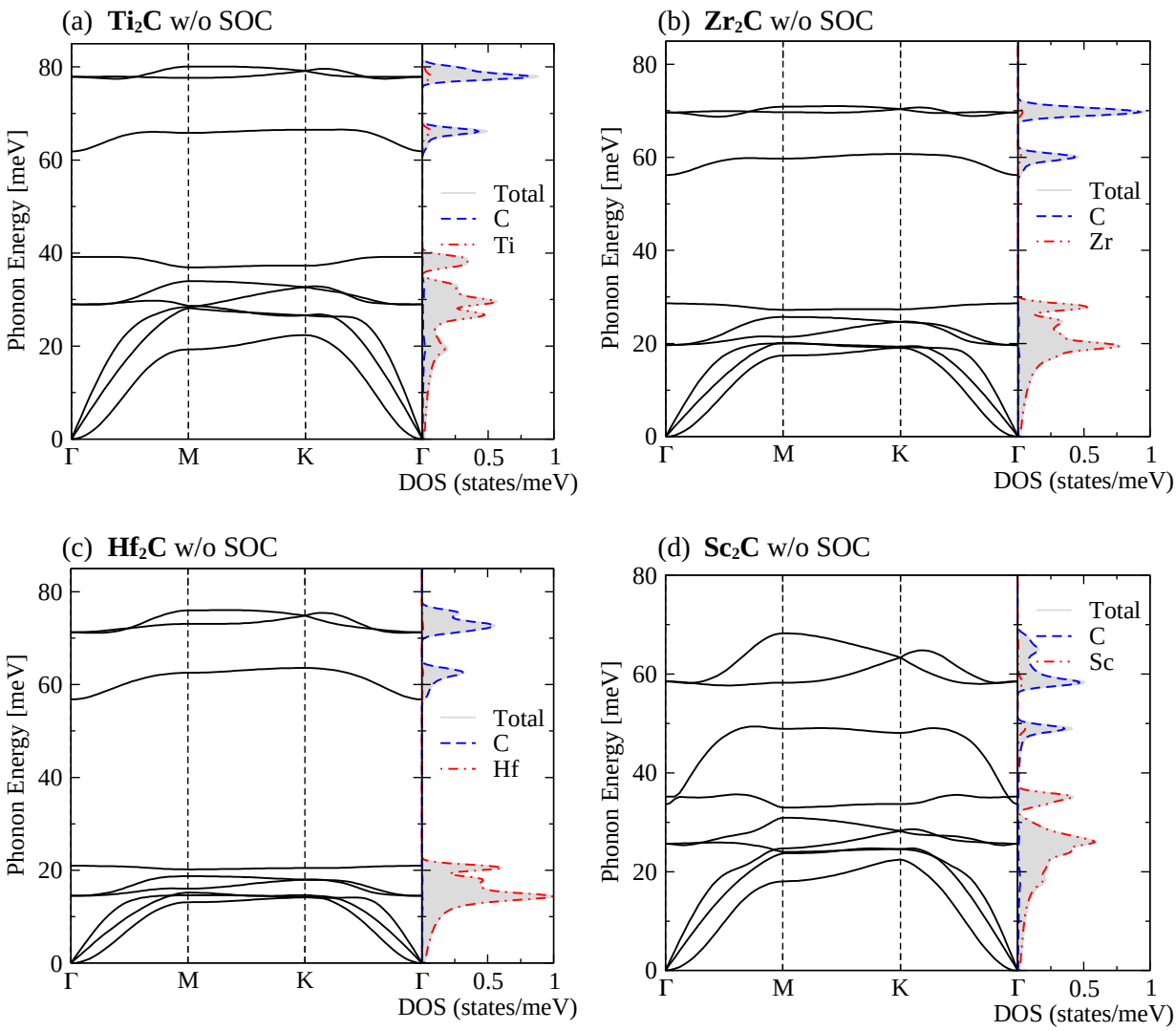

Figure 24: Vibrational spectrum of M_2C (M = Ti, Zr, Hf, Sc) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in states/meV.

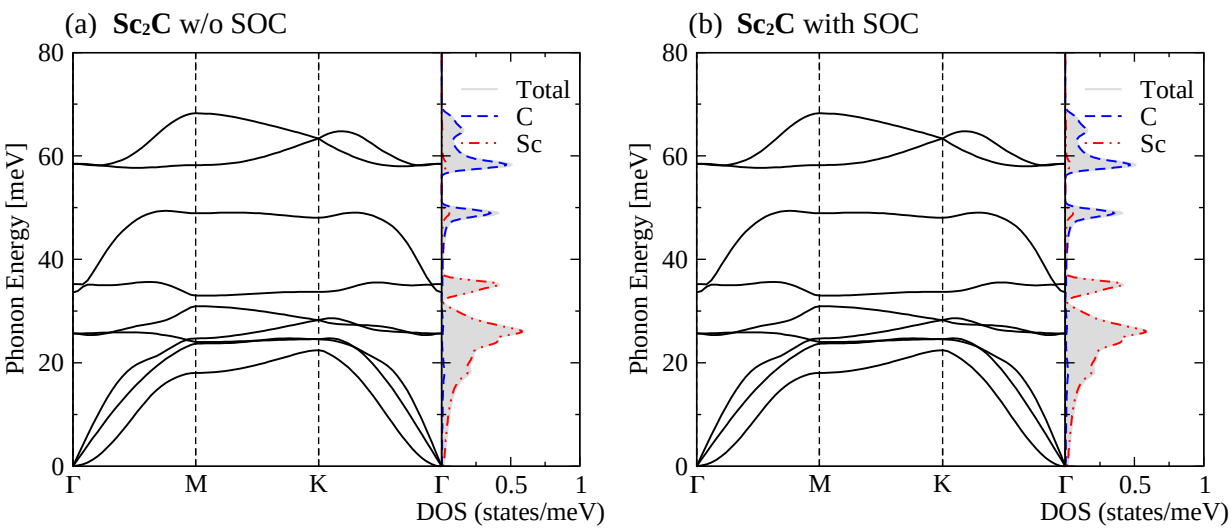

Figure 25: Vibrational spectrum of M_2C (M = Ti, Zr, Hf, Sc) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in states/meV.

PHONON SPECTRUM – NITRIDES

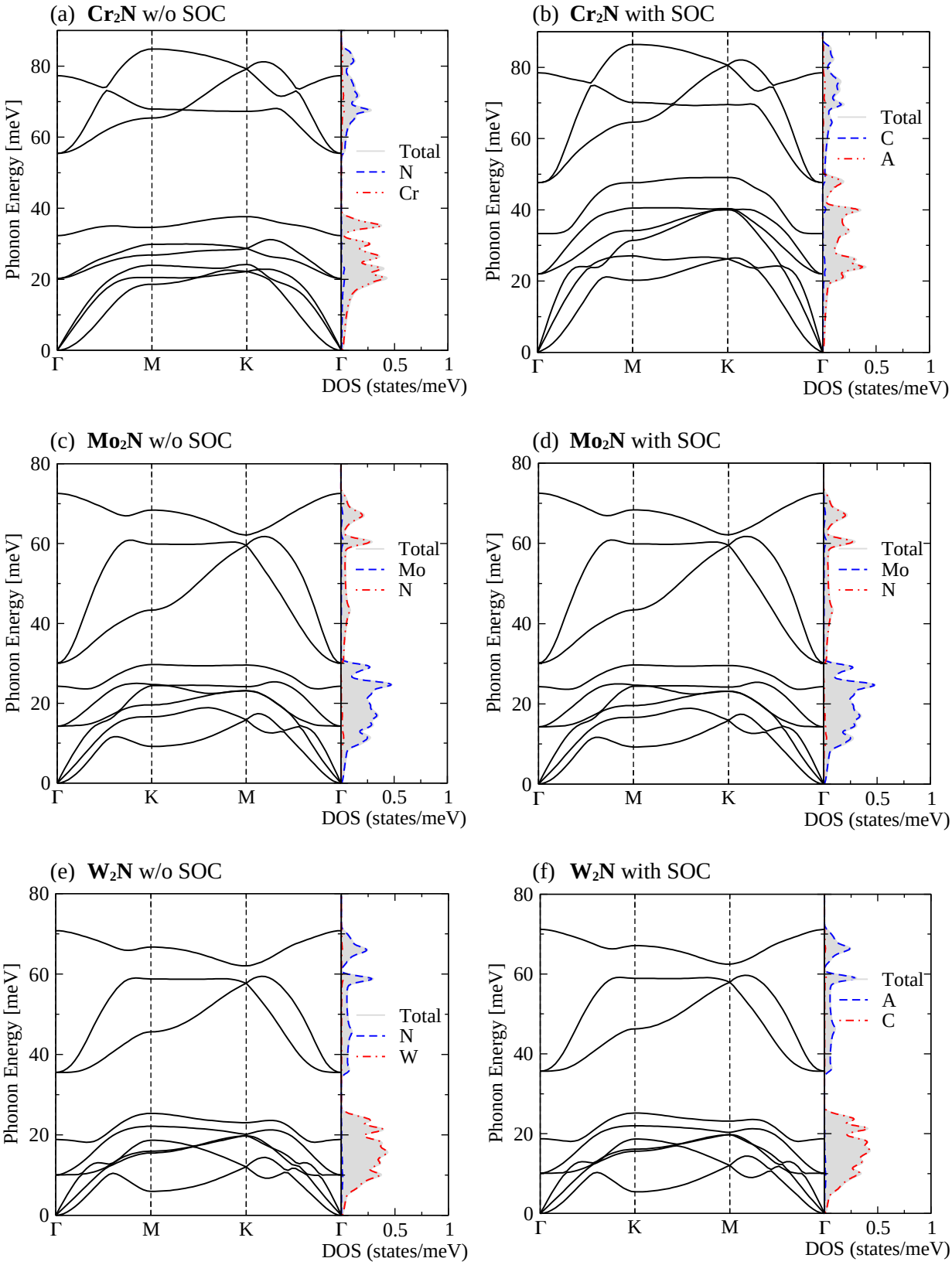

Figure 26: Vibrational spectrum of M_2N (M = Cr, Mo, W) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in states/meV.

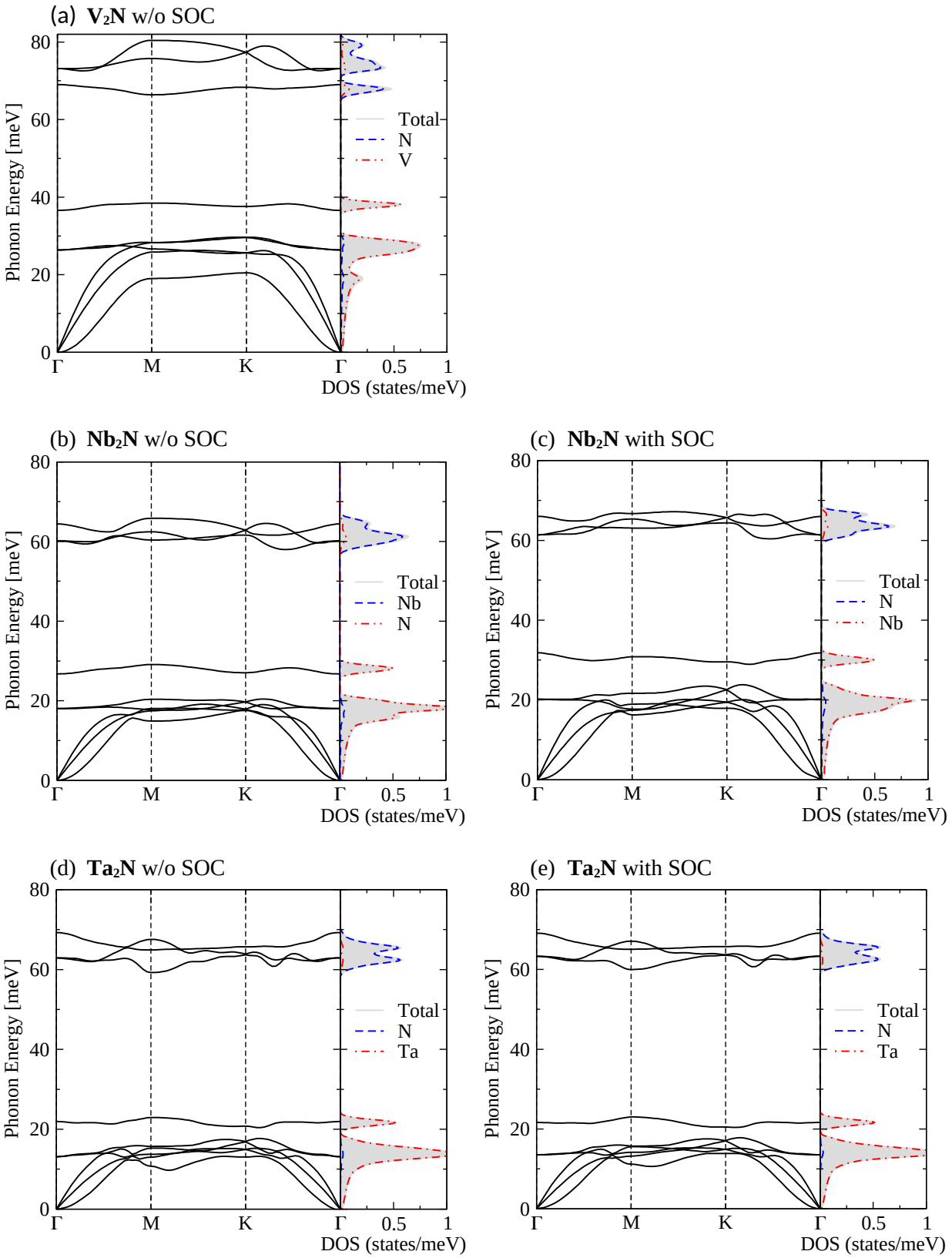

Figure 27: Vibrational spectrum of M_2N (M = Cr, Mo, W) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in states/meV.

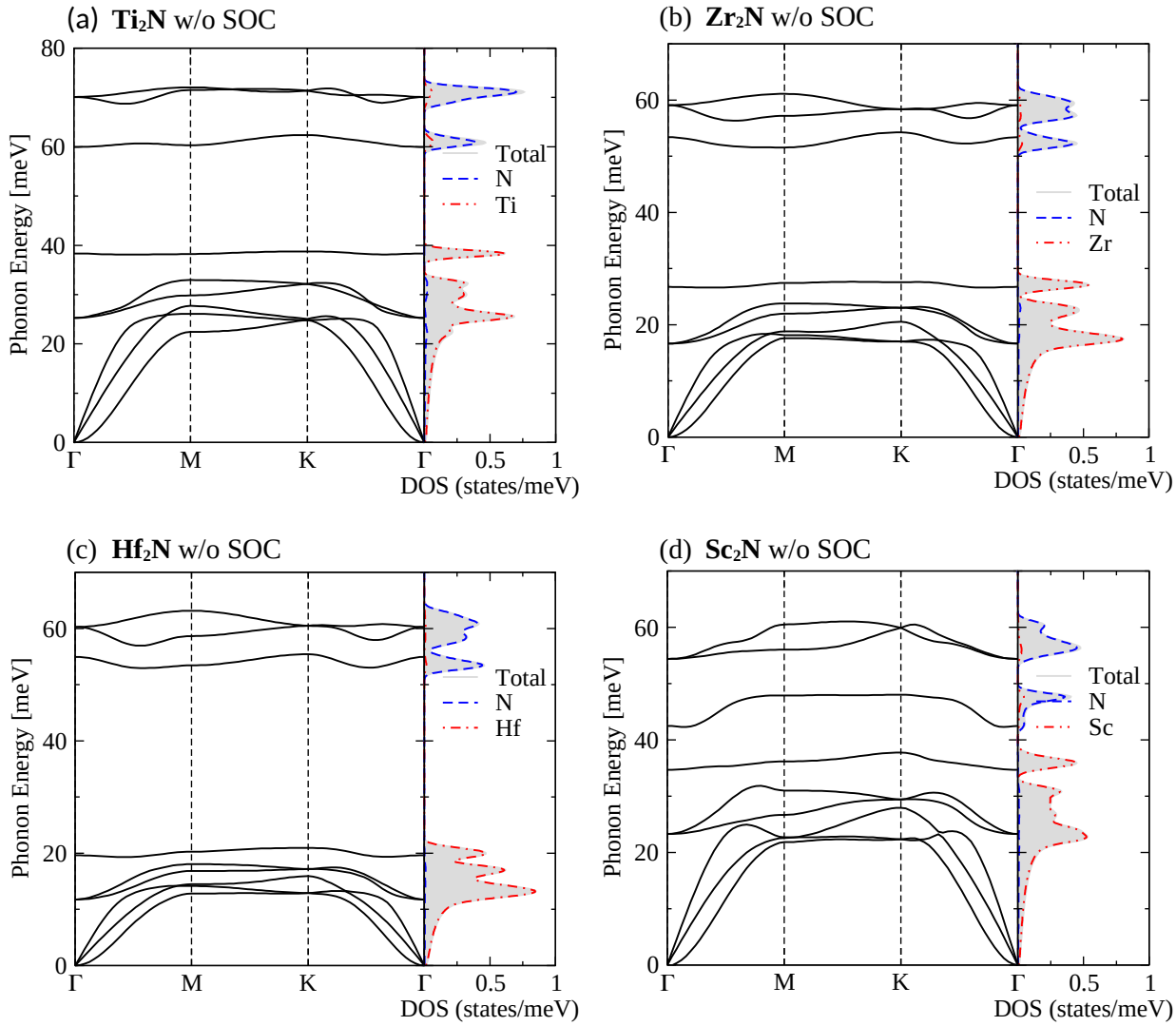

Figure 28: Vibrational spectrum of M_2N (M = Ti, Zr, Hf, Sc) with and without spin-orbit coupling, along the high-symmetry directions of the hexagonal Brillouin zone. DOS in states/meV.