Stability and electronic structure of functionalized 2D molybdenum nitrides - Mxenes

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MXenes are relatively new family of low dimensional materials, which has been gaining more and more popularity in recent years. MXenes are mainly carbides and nitrides of early transition metals and they combine the properties of both components. Bare MXenes typically exhibit metallic behaviour and, therefore, are known to be good electric conductors. Interestingly, this property changes with functionalization of their surfaces. It occurs that functionalizing groups can change metallic Mxenes into semiconducting ones, and not only open the band gap but also influence other properties, just opening the path towards many potential applications, *e.g.*, in electronics, optoelectronics, and thermoelectricity.

In this communication, we present probably the first reported studies of geometry, stability, and electronic structure of bare and functionalized molybdenum nitrides Mo_2N (MXenes). The studies are based on first-principles calculations in the framework of density functional theory (DFT) employing pseudo-potentials and plane-wave basis as implemented in the *QUANTUM ESPRESSO* package. Here, we discuss the results for the bare, and functionalized with oxygen and fluorine Mo_2N layers. All three systems are predicted to be stable at room temperature. The bare Mo_2N is metallic with good electric conductivity. Functionalization of Mo_2N with F leads to opening of the band gap by 0.09 eV and emergence of *n*-type semiconductor, whereas the Mo_2N functionalization with O creates *p*-type semiconductor with energy gap of 0.49 eV.

Further, with the output from the performed calculations, we have started the calculations of physical quantities that determine the thermoelectric properties of these materials.

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