Outstanding Thermoelectric Properties (ZT ≈ 5 – 6) 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, electronic structure and transport properties 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. The bare Mo_2N is metallic with good electric conductivity. Functionalization of Mo_2N with F leads to opening of the band gap of 0.09 eV below the Fermi level, whereas the Mo_2N functionalization with O creates p-type semiconductor with energy gap of 0.49 eV.

The electronic transport properties were calculated using BoltzTraP2 code and the phonon transport properties were obtained by the Phono3py. It occurs that functionalization has significant impact on Seebeck coefficient and lattice thermal conductivity of these materials, quantities strongly determining the thermoelectric performance. The Seebeck coefficient is increased to $2.5*10^{-4}$ VK^{-1} for Mo_2NF_2 and $1.2*10^{-3}$ VK^{-1} for Mo_2NO_2. Functionalization decreases lattice thermal conductivity by about 6.5 times for Mo_2NF_2 and 10 times for Mo_2NO_2. These effects lead to the impressive thermoelectric properties of studied MXenes - with thermoelectric figure of merit in the range of $0.3 < ZT < 0.78$ for Mo_2NF_2 and $2.25 < ZT < 5.65$ for Mo_2NO_2, what outperforms all currently known materials.

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