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Gas adsorption on MXene surfaces: Density Functional Theory calculations

Two dimensional graphene-liked materials, so-called MXenes, have been discovered recently. MXenes are layers of transition metal carbide and nitride compounds. According to their large surface area and their distinctive properties, MXenes are promising materials for many applications such as energy storage, supercapacitor, gas storage and thermoelectric applications. This work investigated gas adsorption on MXenes (i.e. Ti2C, V2C, Nb2C and Mo2C) and their oxygen-functionalized surfaces (O-MXenes) by using the periodic Density Functional Theory (DFT) calculations. The adsorbates are N2, NO, NO2, NH3, CO, CO2, O2, H2, H2S, SO2 and H2O molecules. Both dissociative and molecular adsorption processes were observed depending on adsorption sites, types of MXene and adsorbate molecules. The functional group on the surface also plays an important role in its gas adsorption ability. On bare surfaces, the chemisorption process with high adsorption energy indicates high reactivity of MXene towards gas molecules. In the functionalized cases, O-MXenes show weaker gas adsorption strength than bare MXenes, but they are more selective to particular gas species. The results are useful for applying these materials in gas separation, gas storage and gas sensor applications. Structural and charge analysis were performed for understanding the interaction between adsorbates and substrates.

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