

# Theoretical study of two-dimensional titanium carbide MXenes functionalization process

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MXene phases are a new rapidly developing class of two-dimensional materials with suitable electronic, optical and mechanical properties for different applications [1]-[3]. These phases consist of transition metals such as Ti, Sc, Zr, Hf, V, Nb, Ta, Cr, Mo and carbon or nitrogen atoms, and can be produced through the etching of layered MAX phases. During the etching process, it is possible to terminate the surface by O, OH, and F functional groups in order to modify materials properties [4]-[6]. In this work, we accurately describe the surface distribution of functional groups and its interaction with titanium-based two-dimensional carbides in the solution through the use of different approaches. The free Gibbs energies of formation for the distinctly terminated surfaces have studied by combining DFT, phonon calculations and implicit solvation model. Our results indicate the formation of O, OH and F mixture, which coincides with experimental data [1]. Furthermore, DFT together with cluster expansion (CE), and Monte Carlo methods are employed to investigate the distribution of the functional groups on the surface. The proposed computational approach allows us to deeper understand a functionalization mechanism and introduce the range of experimental conditions for further tuning the MXenes properties.

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