Theoretical study of Ti_2C 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. These phases consist of early transition metals such as Ti, Sc, Zr, Hf, V, Nb, Ta, Cr, Mo and carbon or nitride, and could 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 MXenes's properties. The electrochemistry of etching process is one of the crucial points for further developments and understanding of functionalization mechanisms. Adsorbtion of charged molecules on the surface can change an overall surface charge which causes the repulsive or attractive interactions between terminations and substrate. Better understanding of the functionalization process and selection of appropriate conditions would allow us to adjust properties depending on the need. In this work we focused on the investigation of titanium based two-dimensional carbide Ti_2C using combination of various theoretical modelling methods. DFT together with cluster expansion, and Monte Carlo methods are employed to investigate the distribution of the functional groups on the surface. According to this distribution, thermodynamics quantities such as chemical potentials,free energies, and element concentration of the different phases have studied as well as interaction between distinct charged functional groups with solution molecules and the surface.