Contribution ID : **200** Type : **Poster Presentation**

A DFT Study of CO2 Activation on Subnanometric Ni13 Particles Supported on MXenes.

Nowadays CO2 emissions are one of the most critical aspects of the anthropic fingerprint, from fossil fuels utilization to general byproducts of industrial processes, since It is one of the main greenhouse gases. However, CO2 is also a useful chemical in in many processes1,2: reverse water gas shift, hydrogenation of CO2 to methanol and dry reforming using CO2 and methane to produce H2, which in turns is tremendously useful as clean fuel or chemical reactant. CO2 is an almost inert gas, whose activation is strongly endothermic in every process. The research for materials capable of activating CO2 is thus very active. MXenes are a promising new family of materials that exhibit good properties for adsorbing molecules and metal ions or particles3. They are obtained from the chemical or physical etching of MAX phases, 3D material, to exfoliate the metal carbide or nitride sheet, with surface termination of different nature, depending on the solvent and the chemical used for its etching. Thus, MXenes offer a planar support valid for catalysis exposing two sides, maximizing the reacting surface. Due to their nature and composition, MXenes are versatile materials that have the potential to low costs and complexity of catalysts. Supported transition metal clusters and nanoparticles are the paradigm in heterogeneous catalysis. Nickel, in particular, is widely studied for its capability to activate small molecules, and in particular carbon dioxide. 4 Aim of this study is to characterize the interaction of carbon dioxide with a subnanometric icosahedral Ni13 particle supported on M-Xenes, unraveling the role of the interaction with the support. Preliminary results on the adsorption and dissociation of CO2 reveals a comparable activation, respect analogous models4, in which the CO2 shows an average of bending angle among all possible adsorption configuration (10 configurations) of 130° roughly, with a range of Eads of -0.57 eV. Moreover, the activation barrier is around 0.52 eV, which is comparable and even lower respect some references4.

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