Title: **Width Effect on CO_2 Capture by Carbide MXenes.**

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Nowadays, the global warming is an issue that mankind cannot ignore, as it is causing important changes on the Earth climate. The origin of this greenhouse effect are the raising emissions of carbon dioxide (CO_2), mostly coming from the use of fossil fuels such as coal and petrol. At present, new ways to fight this problem are being studied, *e.g.* by the reduction of CO_2 emissions of industry and the use of renewable energies. Here we focus on a particular strategy where a material collector captures the CO_2 from air. This way, the material converts the CO_2 molecule from an inert linear state to an active, adsorbed, bent molecule, triggered from a substrate charge transfer to the CO_2, eventually enabling its posterior utilization as well.

A new family of layered materials, called MXenes, have been proposed for such CO_2 capture. MXenes follow a $M_{n+1}X_n$ in (n=1,2,3) formula, with X=C or N. The thinnest versions of M_2X stoichiometry have been proposed for the CO_2 capture based on first principles simulations. Here we extended the study to the 5- and 7- layered ones, analyzing whether the CO_2 capture capabilities are kept, studying so by Density Functional Theory (DFT) simulations.

The results, including the fundamental vibrational energy and a proper description of dispersive forces, show that these latter energies contribute stabilizing the CO_2 although the effect is mild. In general terms, when increasing the MXene width, the CO_2 still gets activated, showing a bent molecular structure, with elongated C-O bonds, and becomes negatively charged. The maximum interaction is found for the 5-layered MXenes, which point its stoichiometry and/or a particular electronic structure as possible key factors in the enhanced adsorption of CO_2 upon.

Keywords: Carbide MXenes, Density Functional Calculations, CO_2 capture, Environmental Science.