Title: **Width Effect on CO_2 Capture by Nitride MXenes**
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SUMMARY

The greenhouse effect that occurs when gases in the atmosphere keep warm of the solar radiation is the cause of the global warming and the climate change. The main responsible is CO_2 which has raised due to anthropogenic emissions, e.g. by the combustion of fossil fuels. The global warming can have more effects, including the acidification of the Earth's oceans. Nowadays there are many strategies to reduce the CO_2 emissions or to reduce the concentration of CO_2 in the air.

Capturing, storing, and activating CO_2 on transition metal nitrides surfaces has been proposed as feasible route to the latter. This new class of two-dimensional (2D) materials called MXenes with the formula $M_{n+1}N_n$, and a large surface area of contact, where M = Ti, V, Cr, Zr, Nb, Mo, Hf, Ta, W, and X = C, N, and layers of C or N are intercalated between metallic layers. These has potential use for capturing CO_2. In this sense it is interesting to investigate whether CO_2 capture is biased by the MXenes stoichiometry, which also means, increasing their width, i.e. whether it is affected by using 3, 5, and 7 atomic layers of the MXene materials.

This study will be carried out using computational calculations based on Density Functional Theory (DFT),[1] including dispersive forces, showing that these systems are capable of capturing and activating CO_2 in their more stable surface, as analyzed from the distances, angles, and the charge transferred to CO_2 getting information about the CO_2 strong interaction.

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