Title: **Carbide MXenes Surface Tensión Effect on CO_2 Capture**

Student: Daniel Dolz Garcia

Date: July 2020

Supervisor/s: Dr. Francesc Viñes Solana
Department of Material Science and Physical Chemistry

Dr. Ángel Morales García
Department of Material Science and Physical Chemistry

One of the major challenges of our nowadays society is the fight against climate change derived from the gradual global warming of the Earth surface due to the high concentration of detrimental greenhouse gases in the atmosphere, such as CO_2 or CH_4. These gases absorb the radiated heat emitted by the Earth toward space consequently promoting the so-called greenhouse effect. In principle, this effect is beneficial, because it leads to the thermal stability that is essential for life. However, the anthropogenic activity has derived into a great dependency of fossil fuels, especially since the industrial revolution, generating an excessive concentration of the above-mentioned gases, and so increasing the Earth temperature leading as well to the acidification of oceans. Nowadays, the CO_2 concentration in the atmosphere has reached 360 ppm, and this amount is expected to be doubled by the end of this century. The direct consequence of such concentration is the increase of the Earth's temperature, expected to rise 2-5 ºC, leading to the melting of the poles, augmenting the level of the sea, and causing floods and other devastating phenomena across the world. To minimize, even avoid such consequences, new technologies are sought to reduce these greenhouse gases concentrations.

The usage of CO_2 sweeper derived materials emerges as a suitable technology for Carbon Capture and Storage (*CCS*). In this context, Transition Metal Carbides (*TMCs*) materials have been suggested as potential substrates for CO_2 capture and activation due to the exothermic CO_2 adsorption even at low partial pressures. Interestingly, the two-dimensional counterparts of TMCs, called MXenes, have shown an even better performance for CCS. These MXenes are synthetized by MAX phase precursors exfoliation techniques, thus depending on the MAX phases composition and demanding a certain energy to foster the layers separation. Indeed, such an exfoliation energy could be a descriptor to seize the resulting MXene chemical activity, here analyzed in depth through computational simulations, correlating the CO_2 adsorption energies on MXenes with the estimates of exfoliation energies.

Keywords: MAX Phases, MXenes, Density Functional Calculations, CO_2 capture, Environmental Science