Ángel Morales-García
Francesc Viñes, Raúl Morales-Salvador, Francesc Illas
Departament de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, c/ Martí i Franquès 1-11, 08028, Barcelona, Spain.

angel.morales@ub.edu

CO_2 chemical trapping on two-dimensional MXenes

Carbon dioxide (CO_2) concentration in the Earth atmosphere is a critical issue since it is behind the greenhouse effect, global warming, and oceans acidification. The need to reduce the CO_2 amount in the atmosphere has triggered diverse research into CO_2 sequestration, also oriented towards its ulterior utilization as a chemical feedstock in the chemical industry. Therefore, CO_2 chemical trapping on active solid-substrates emerges as one of the most feasible routes for this purpose. The so-called carbon capture and storage (CCS) strategy requires specific solid substrates that are able to absorb CO_2 in a sufficiently strong way. However, CO_2 adsorption on most solid surfaces is very weak, which constitutes CCS a real challenge. Inspired by recent work on the CO_2 adsorption on transition metal carbides [1] and by the discovery of an entirely new family of two-dimensional (2D) transition metal carbides and nitrides, termed MXenes [2], with general $M_{n+1}X_n$ chemical formula (M stands for an early transition metal, and X for C or N), we launched a systematic study to inspect whether these new 2D materials provide promising candidates for efficient CO_2 abatement.

Hereby, we will present results for adsorption/desorption rates derived from state-of-the-art density functional theory (DFT) based calculations including dispersion, coupled to transition state theory (TST). The present results strongly suggest that these 2D M_2C and M_2N materials (M=Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, and W) have a great potential for CO_2 storage and activation. This claim is supported by calculated high adsorption energies, ranging from -1.03 to -3.69 eV, and a significant MXene→CO_2 charge transfer. Adsorption and desorption rates derived from TST predict that these materials can adsorb CO_2 up to elevated temperatures and low partial pressures, with CO_2 uptakes ranging from 2.32 to 8.25 mol CO_2 kg^{-1} of substrate, quite competitive to other nowadays-existent material solutions [3,4]. Our predictions have been confirmed experimentally showing single sheets of Ti_3C_2 MXene as a potential solid adsorbent for carbon capture applications [5].

References

[1] C. Kunkel, F. Viñes, F. Illas, Energy Environ. Sci., 9 (2016) 141-144.
[2] B. Anarosi, M. R. Lukatskaya, Y. Gogotsi, Nat. Rev. Mater., 2 (2017), 16098 (1-17).
[3] A. Morales-García, A. Fernández-Fernández, F. Viñes, F. Illas, J. Mater. Chem. A., 6 (2018) 3381-3385.
[4] R. Morales-Salvador, A. Morales-García, F. Viñes, F. Illas, Phys. Chem. Chem. Phys., 20 (2018) 17117-17124.
[5] I. Persson, J. Halim, H. Lind, et al., Adv. Mater. (2018) DOI: 10.1002/adma.201805472.

Figures

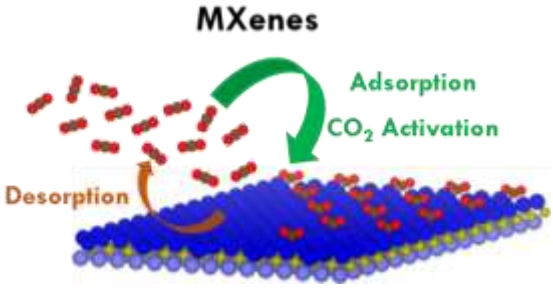

Figure 1: Scheme of the CO_2 chemical trapping on M_2X (X=C, N) MXenes.