Unveiling the Potential of Functionalized 2D Janus MXenes

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Janus MXenes are a class of two-dimensional materials (2D) that exhibit unique structural and chemical properties. They consist of atomically thin layers with a Janus-like structure, meaning that one side of the layer has different chemical elements or functional groups compared to the other side. This structural asymmetry grants them diverse applications, such as energy storage, catalysis, sensing, and electronic devices, making them highly promising in the field of nanotechnology.

I will show how the Sc_2C MXene family seems to be particularly suitable to maximize the performance of nanoelectronic devices in, at least, two different aspects. Through Density Functional Theory calculations, we have explored the mechanical, electronic and magnetic properties of 36 functionalized Sc_2CXT (X = O, F, OH; T = C, N, S) MXenes, revealing interesting aspects such as ferro or anti-ferromagnetism and half-metallicity, depending on the functionalization. On the other hand, the functionalization of Sc_2CX with N_2, ON, or O_2 groups shows competitive performance in terms of Na adsorption, diffusion, and capacity s as anodes for Na-ion batteries (NIBs).

These findings highlight the remarkable potential of Sc_2CX MXenes for various applications in 2D nano-, spin-, and energy-related fields.

References

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[2] S. Özcan and B. Biel, *Phys. Chem. Chem. Phys.* **25** (2023)1881-1888
[3] S. Özcan and B. Biel, *J. Appl. Phys.* **133** (2023) 044301

Figures

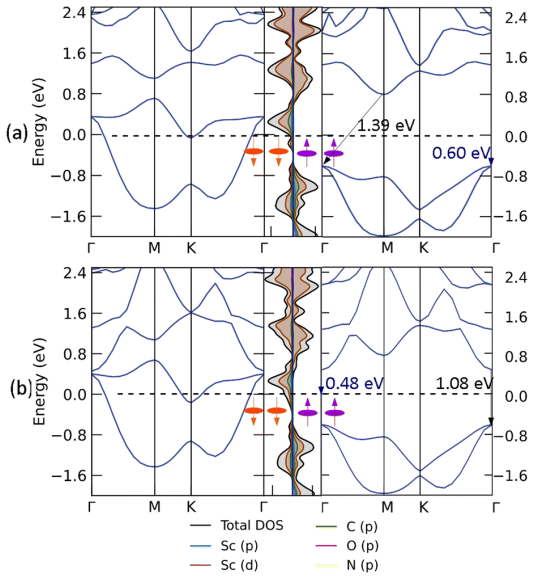

Figure 1: Band and spin-resolved density of states structures of (a) Sc_2CFC and (b) Sc_2COHC.

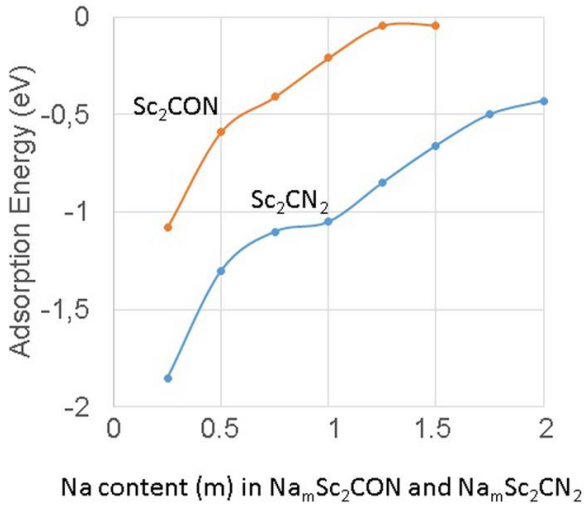

Figure 2: Variation in the adsorption energy with increasing Na content on Sc_2CN_2 and Sc_2CON.