Journal Name

ARTICLE TYPE

Cite this: DOI: 00.0000/xxxxxxxxxx

Interplay of Redox, Double-Layer, and Quantum Effects Governing the Capacitance in Nitrogen-Doped Ti_2CT_x MXene-Based Supercapacitors†

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1 Density of States Calculations Using Hybrid Functional (HSE06)

To examine the influence of doping on the electronic structure of Ti_2CO_2 MXene, hybrid-functional density-of-states (DOS) calculations were carried out using the HSE06 functional for the pristine system, as well as for 10% lattice-site (LS)-doped and 10% functional-site (FS)-doped configurations. These HSE06 calculations complement and validate the electronic structure results based on PBE presented in the main manuscript.

The convergence criteria and computational parameters required to reproduce the results shown in Table 1 of the main manuscript. Large computational files and additional technical details related to these HSE06 calculations are provided in the associated GitHub repository.

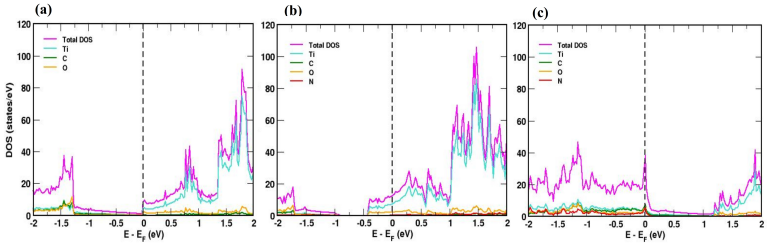

Fig. 1 Density of states (DOS) of pristine Ti_2CO_2 MXene and 10% lattice-site (LS)- and 10% functional-site (FS)-doped configurations calculated using the hybrid HSE06 functional.

The HSE06 DOS results clearly demonstrate that the doping site plays a crucial role in determining the electronic structure of Ti_2CO_2. Compared to the pristine MXene, both LS- and FS-doped configurations exhibit noticeable shifts in the Fermi level and modifications in the conduction-band features, indicating doping-induced changes in the electronic states near the Fermi energy. While the hybrid functional introduces quantitative corrections to the band positions, the overall trends observed are consistent with those obtained from PBE calculations, thereby reinforcing the reliability of the predicted doping effects on the electronic properties of Ti_2CO_2.

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