Supporting Information for:

Article

CO_2 and H_2O coadsorption and reaction on the low-index surfaces of tantalum nitride (Ta_3N_5): a first-principles DFT-D3 investigation

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This supporting information contains the relaxed structures of all possible adsorption CO_2 geometries on Ta_3N_5 (001), (010), and (110) surfaces.

Figure S1: Different possible adsorption geometries of CO_2 on Ta_3N_5 (001) surface

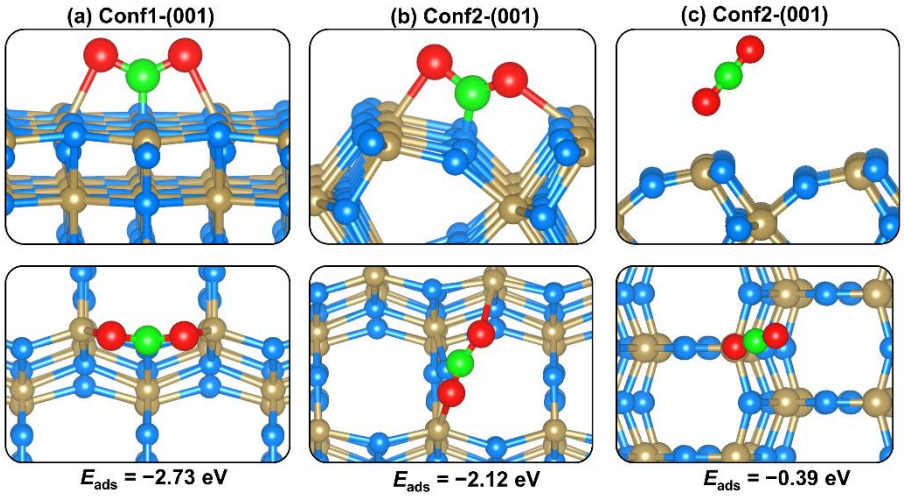

Figure S2: Different possible adsorption geometries of CO_2 on Ta_3N_5 (010) surface

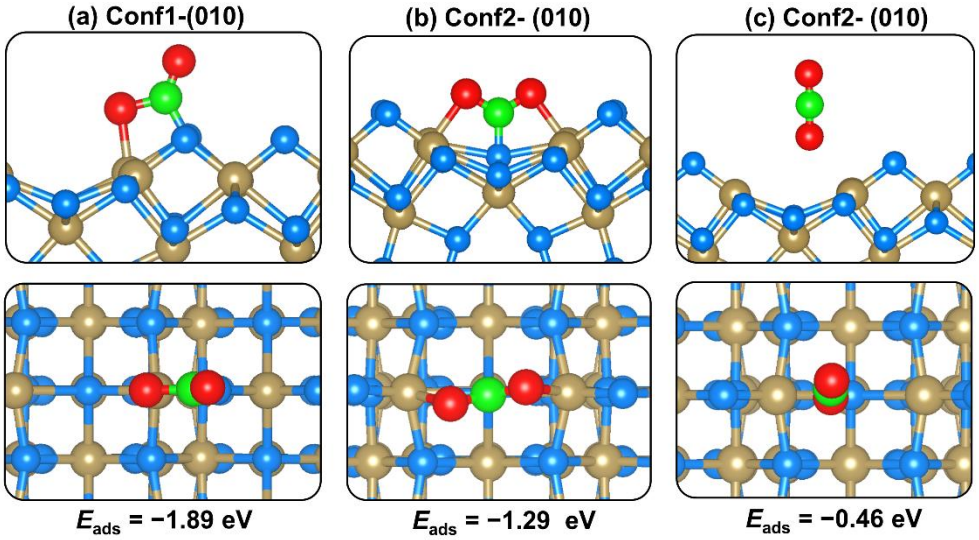

Figure S3: Different possible adsorption geometries of CO_2 on Ta_3N_5 (110) surface