Supplementary Material: CO_2 Capture, Activation and Dissociation on Ti_2C Surface and Ti_2C MXene: Role of Surface Structure

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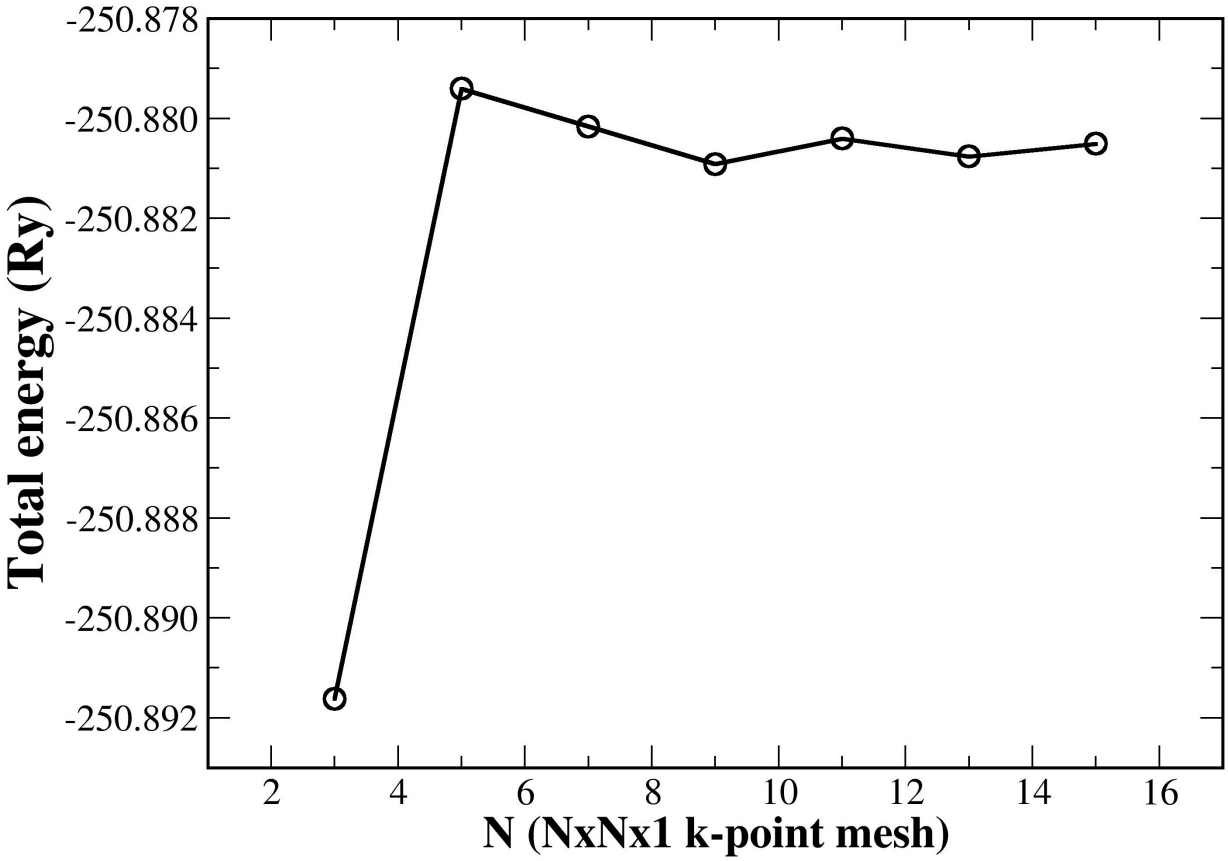

FIG. S1. k-point convergence plot for Ti_2C MXene surface.

TABLE S1. Relative energies of the different magnetic configurations of Ti_2C MXene.

Magnetic configuration	Relative energy (meV/f. u.)
Antiferromagnetic (AFM)	0.00
Ferromagnetic (FM)	33.00
Non magnetic (NM)	142.00

TABLE S2. Relative energies for different magnetic configurations of chemisorbed CO_2 on Ti_2C MXene.

Configuration **5** (Fig. 6 of the manuscript) (Fig. 6 of the manuscript)		Configuration **6** (Fig. 6 of the manuscript) (Fig. 6 of the manuscript)	
Magnetic configuration	Relative energy (eV)	Magnetic configuration	Relative energy (eV)
AFM	0.00	AFM	0.00
FM	0.12	FM	0.23
NM	0.81	NM	0.93

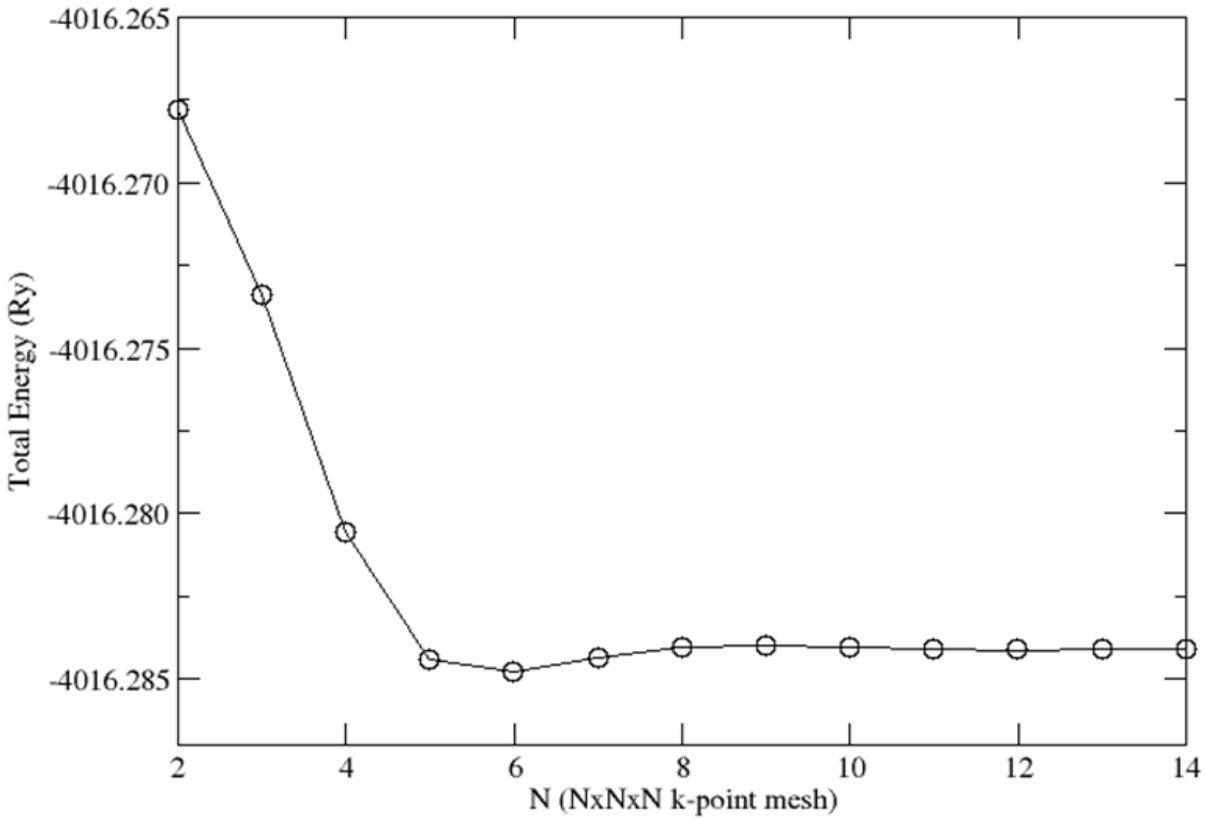

FIG. S2. k-point convergence plot for Ti_2C surface.

TABLE S3. Adsorption energy of CO_2 on magnetic and non-magnetic $Ti_2C\{100\}$ surfaces. All energies are given in eV.

surfaces	E_{mag}	$E_{non-mag}$	E_{diff}
14	-0.29	-0.29	0.0
15	-0.07	-0.07	0.0
16	-0.09	-0.09	0.0
17	-0.04	-0.04	0.0
18	-4.39	-4.39	0.0

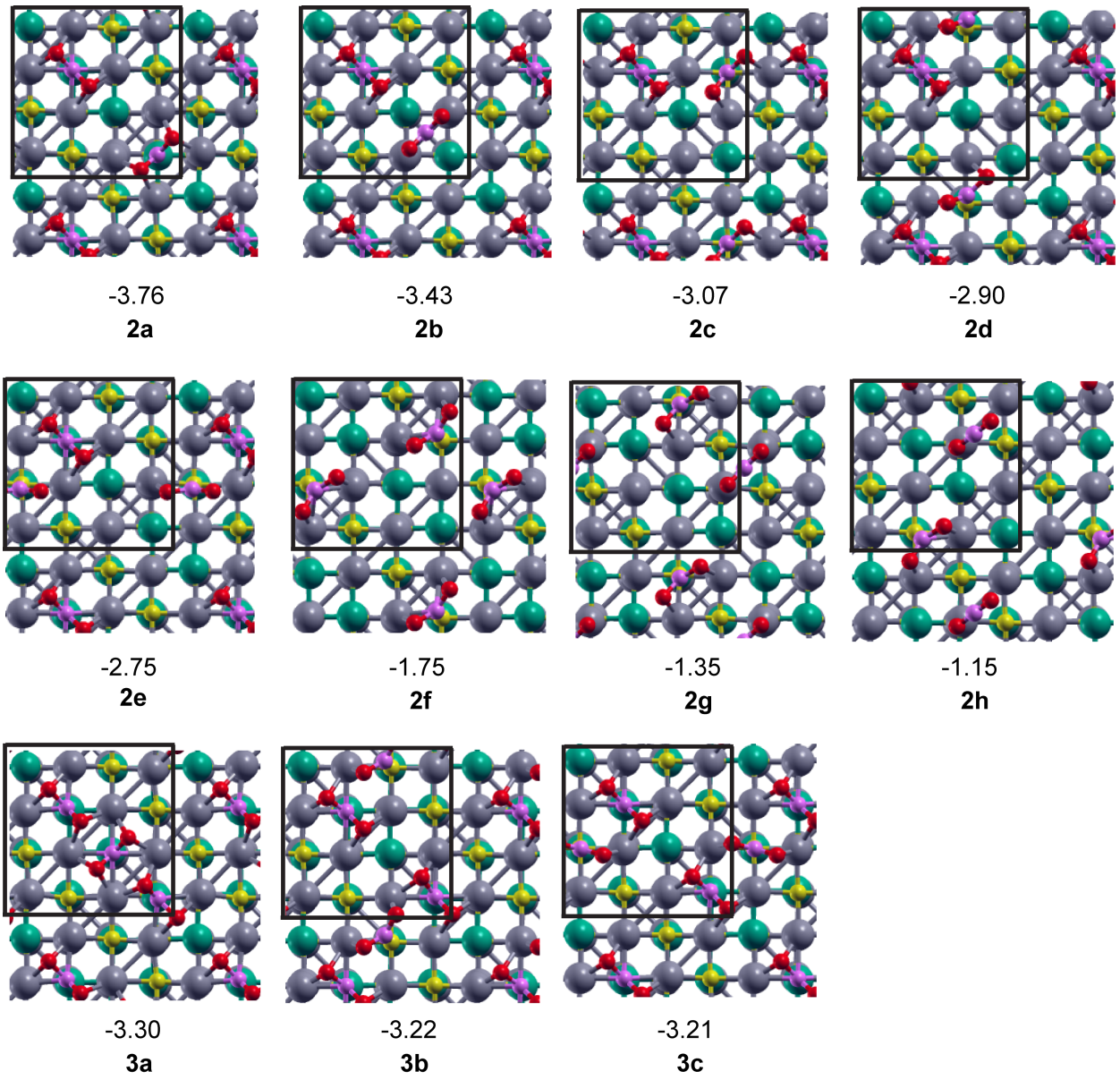

FIG. S3. Geometric variants corresponding to the adsorption of two (geometries **2a**-**2h**) and three (geometries **3a**-**3c**) CO_2 molecules on $Ti_2C\{100\}$ surface; adsorption energy given in eV/CO_2.

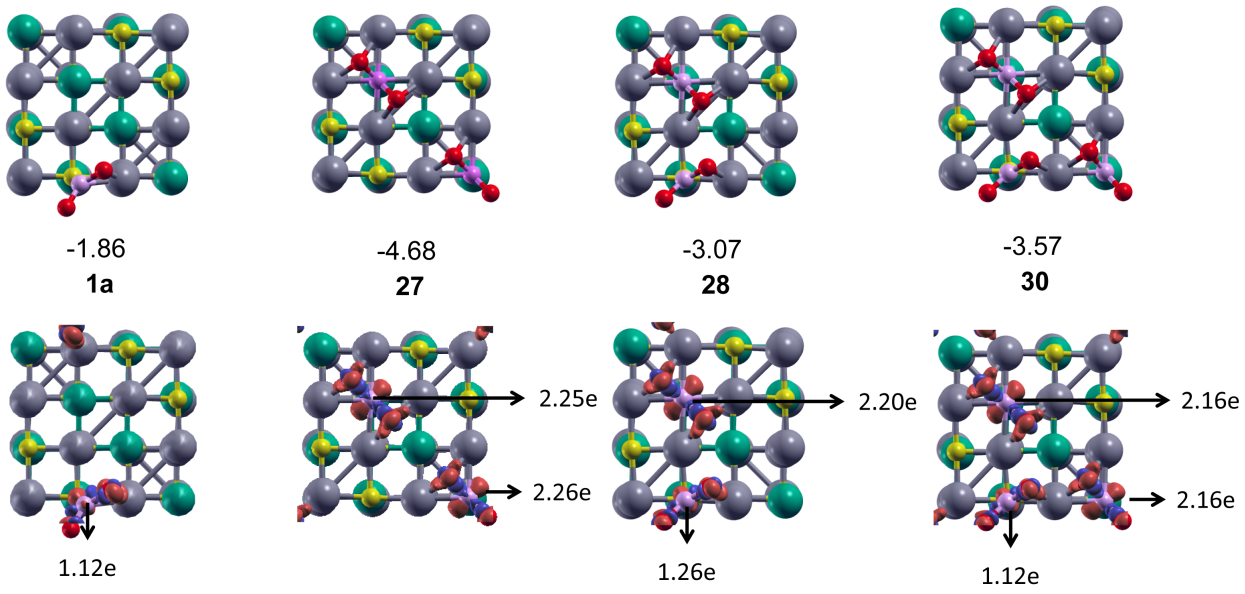

FIG. S4. Charge transfer plots for structures **27**, **28**, and **30**.

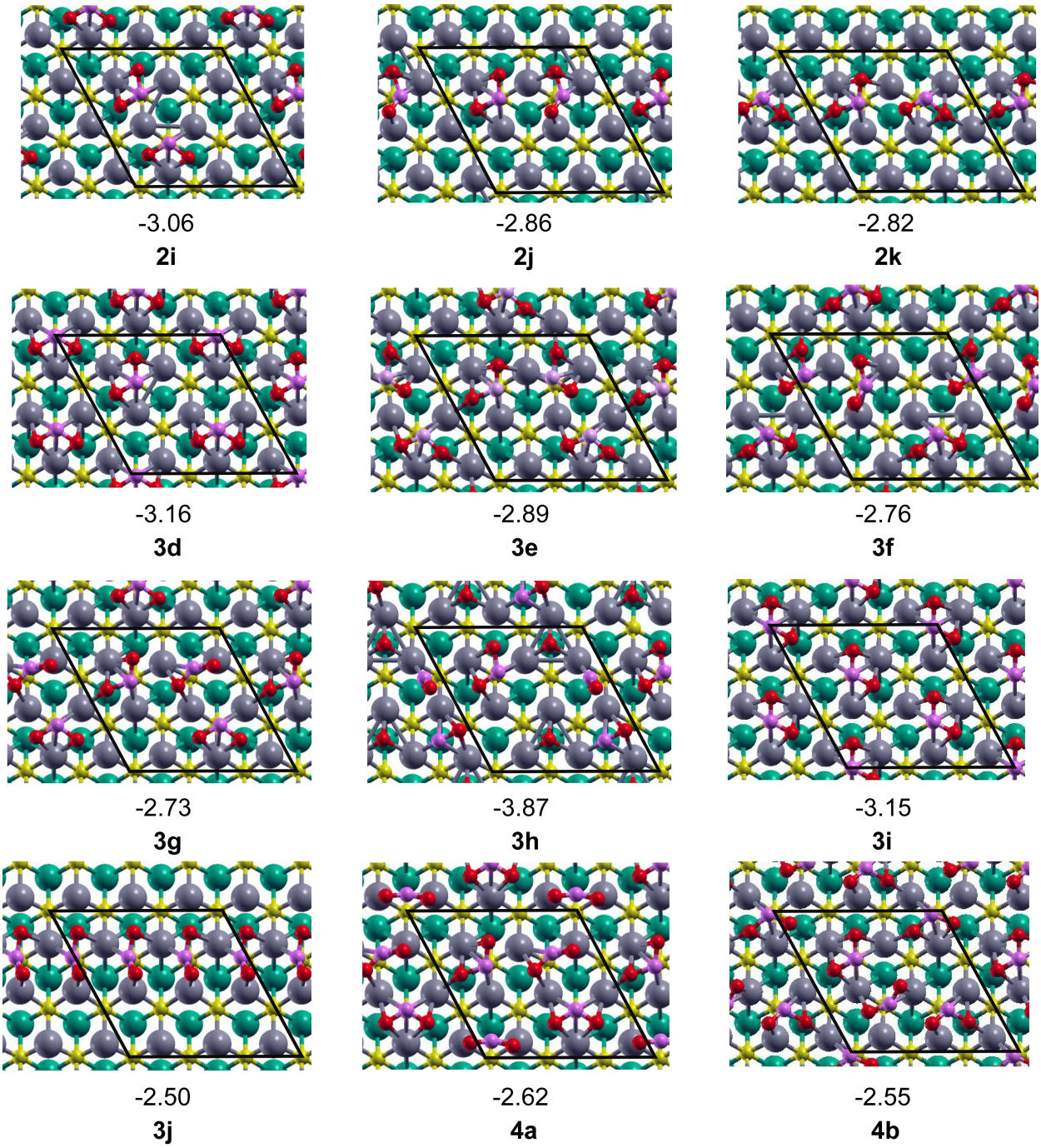

FIG. S5. Geometric variants corresponding to the adsorption of two (geometries **2i**-**2k**) three (geometries **3d**-**3j**), and four (geometries **4a** and **4b**) CO_2 molecules on MXene surface; adsorption energy given in eV/CO_2.

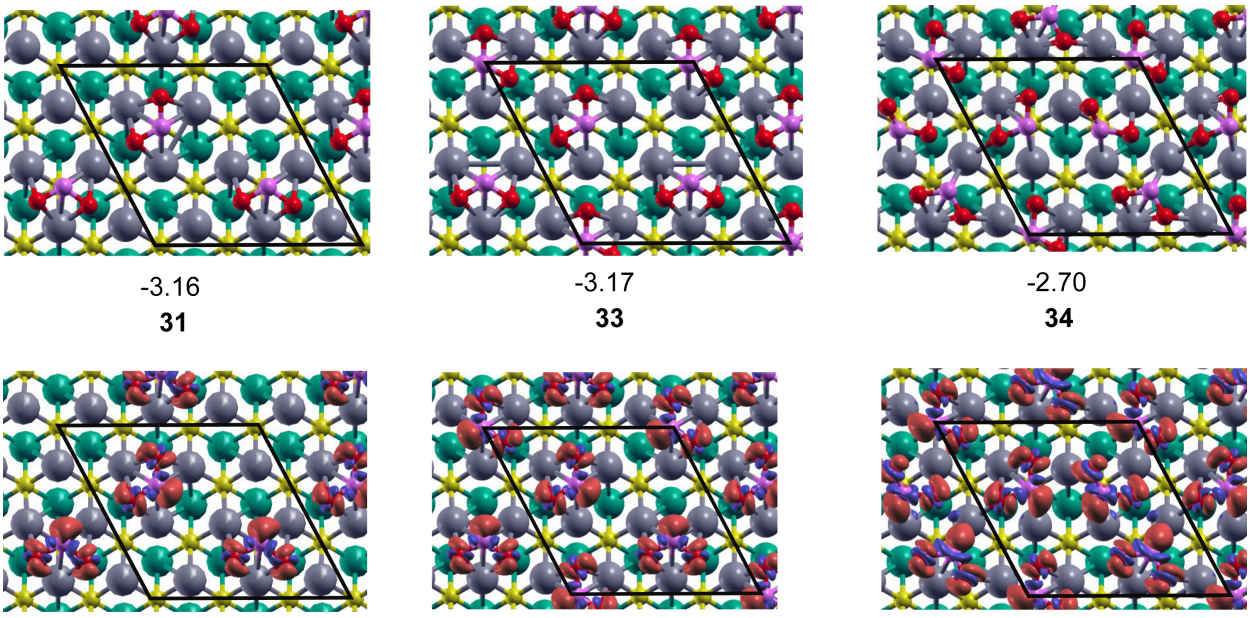

FIG. S6. Charge transfer plots for structures **31**, **33**, and **34**.