

RESEARCH ARTICLE

A DFT study of $\text{Ti}_3\text{C}_2\text{O}_2$ MXenes quantum dots supported on single layer graphene: Electronic structure and hydrogen evolution performance

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Received September 21, 2020; accepted January 4, 2021

SUPPLEMENTARY MATERIAL

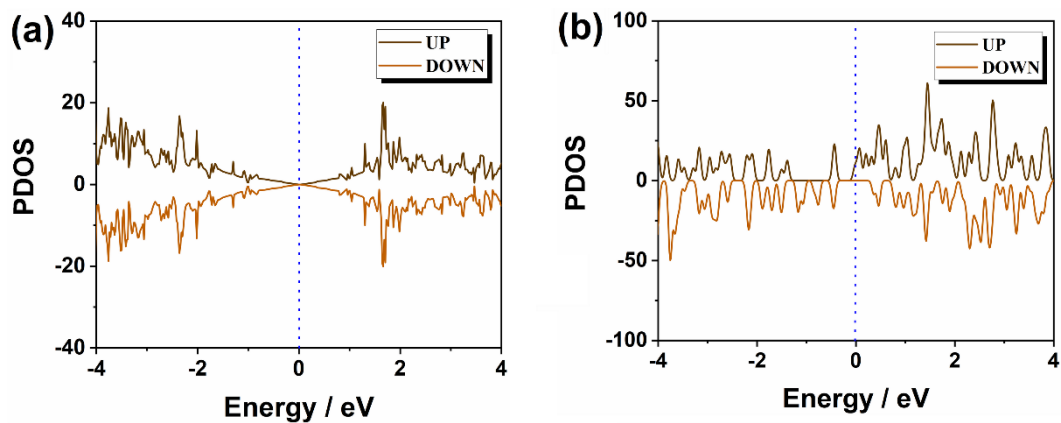


Fig. S1 PDOS of Graphene (a) and $\text{Ti}_3\text{C}_2\text{O}_2$ QDs (b), respectively. Fermi levels are set at 0 eV.

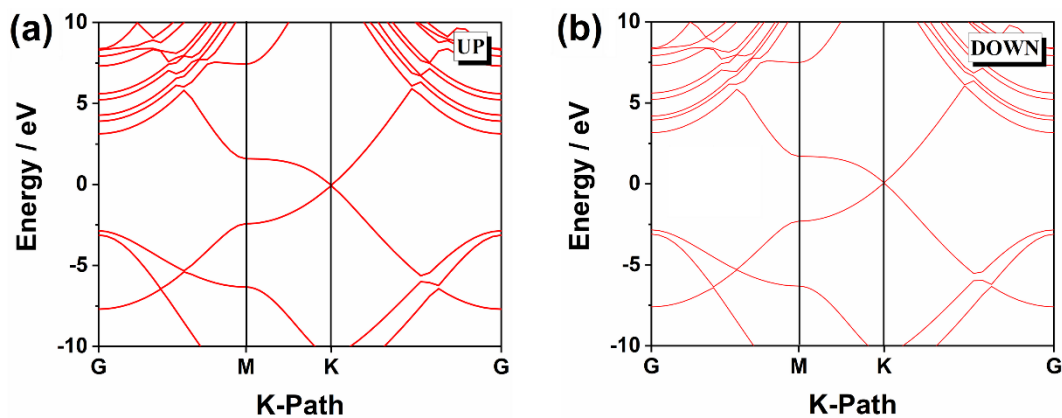


Fig. S2 Band structure of Graphene. Fermi levels are set at 0 eV.

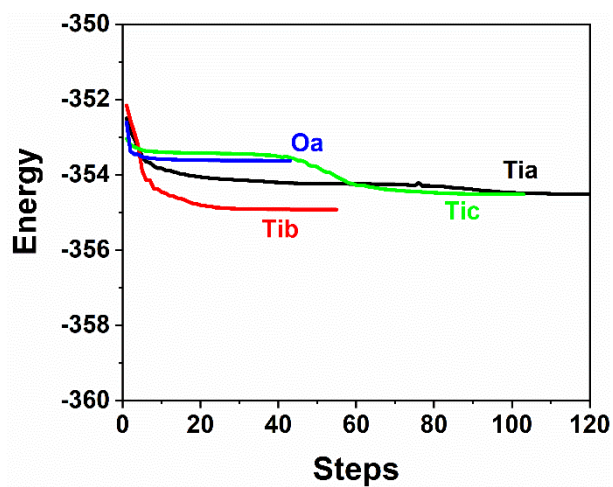


Fig. S3 Energy change during geometry optimization for $\text{Ti}_3\text{C}_2\text{O}_2$ QDs.

Table S1 Zero point energy for H adsorbed on the surface of $\text{Ti}_3\text{C}_2\text{O}_2$ QDs and $\text{Ti}_3\text{C}_2\text{O}_2$ QDs/G heterostructure.

System	E_{ZPE} (eV)
Tia	0.17
Ca	0.24
Oa	0.29
Q-G Tia	0.13
Q-G Tia'	0.13
Q-G Ca	0.24
Q-G Oa	0.29
Q-G Oa'	0.29