

Supporting Information

Theoretical study on lithium storage performance of V-doped Ti_2CO_2 MXene

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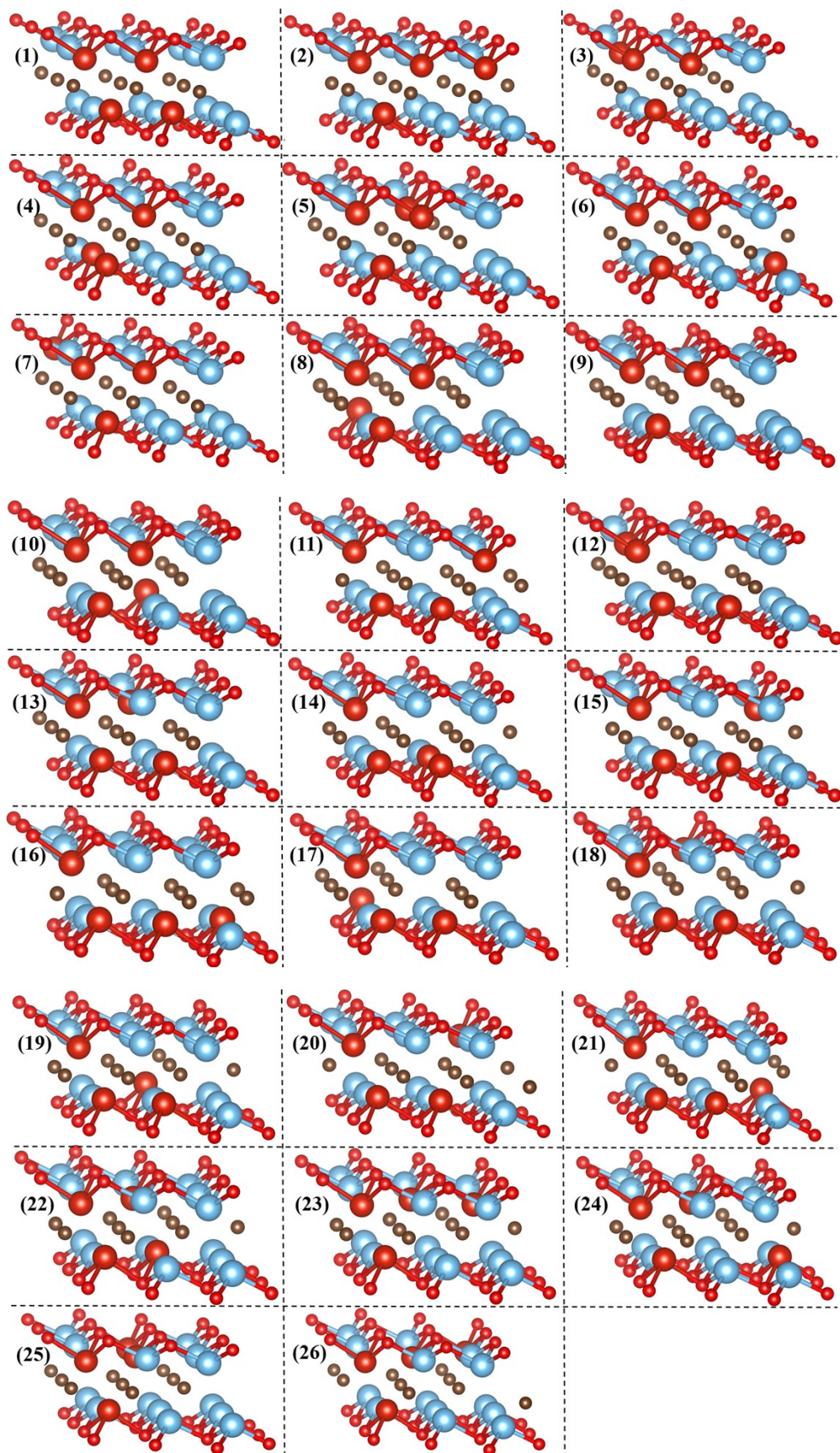


Fig. S1 26 predicted structures of TiVCO₂

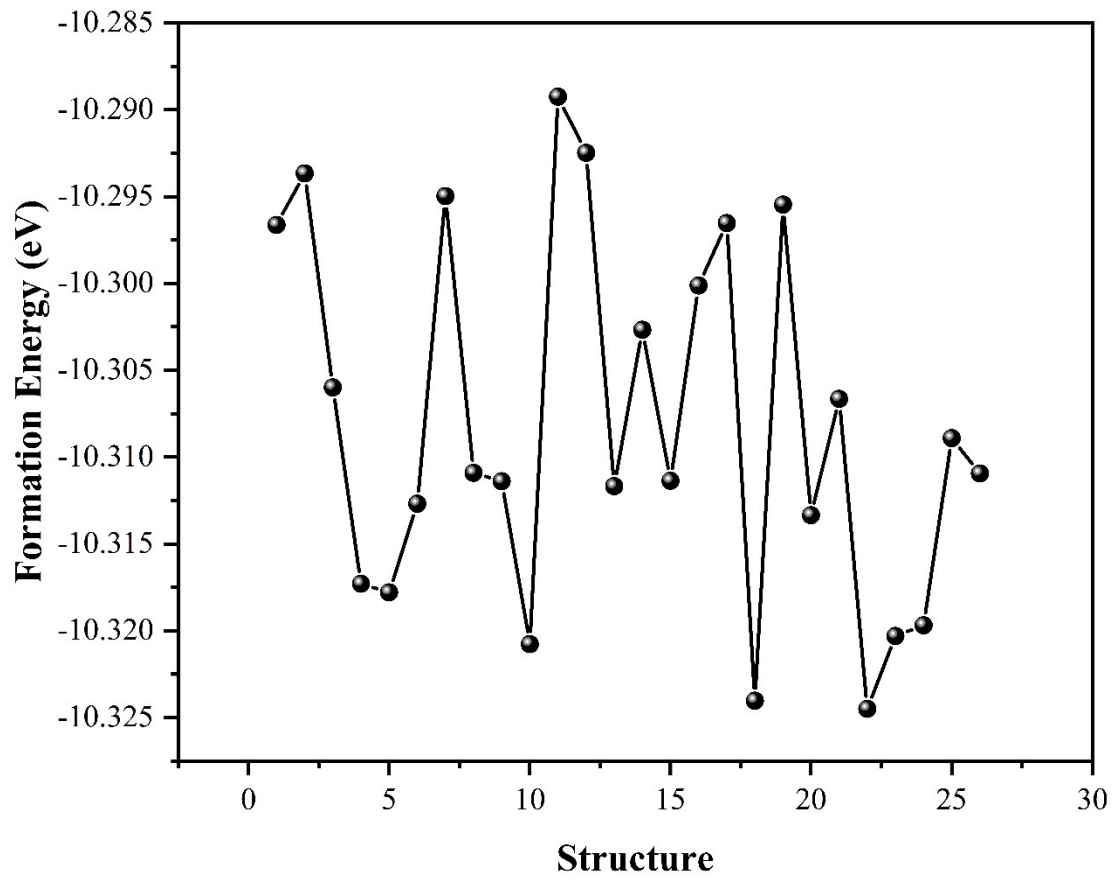


Fig. S2 Formation energy of different predicted structures

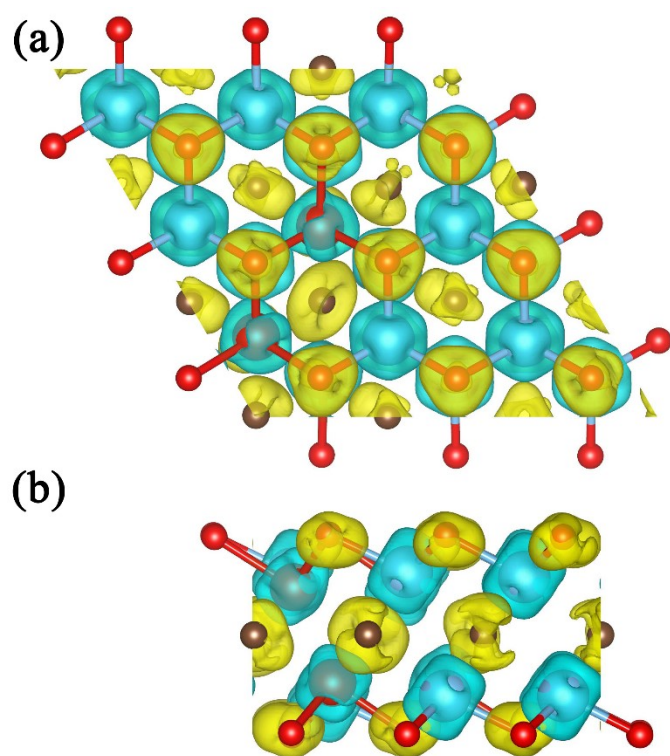


Fig. S3 Top (a) and side (a) view of TiVCO₂ charge density difference.