## Supplementary Material: Oxygen functionalized TITe buckled honeycomb from first-principles study

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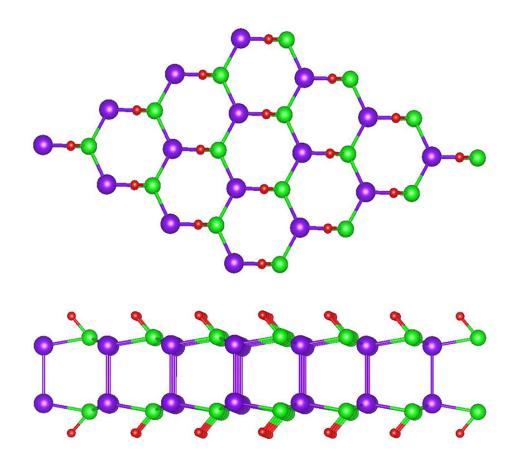


Fig. S1. Snapshots of atomic configuration at 2 ps for TITeO at the end of MD simulation.

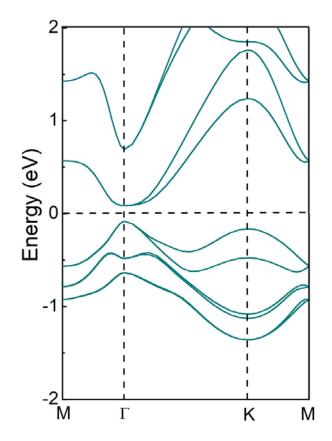


Fig. S2. The band structure of TITeO by HSE06 with SOC.