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# Supporting Information : Theoretical calculation of electrocatalysts properties of freestanding low dimensional $PbTiO_3$ for hydrogen evolution reactions

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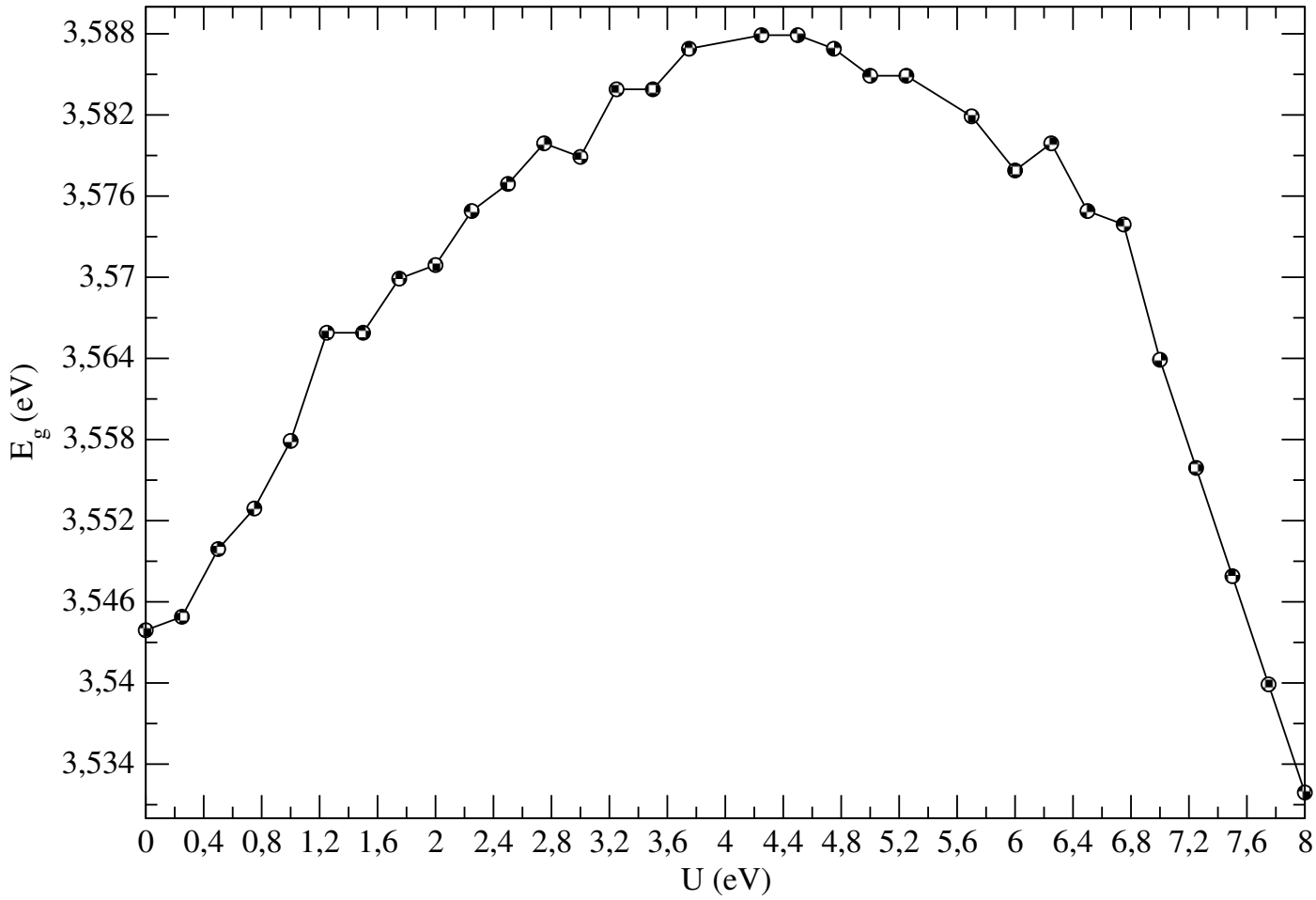


Fig. S1 (Color online) The optimization of Hubbard correction U as a function of band gap $E_g$. Here Hund's corrections $J$ is taken constant at 2 eV

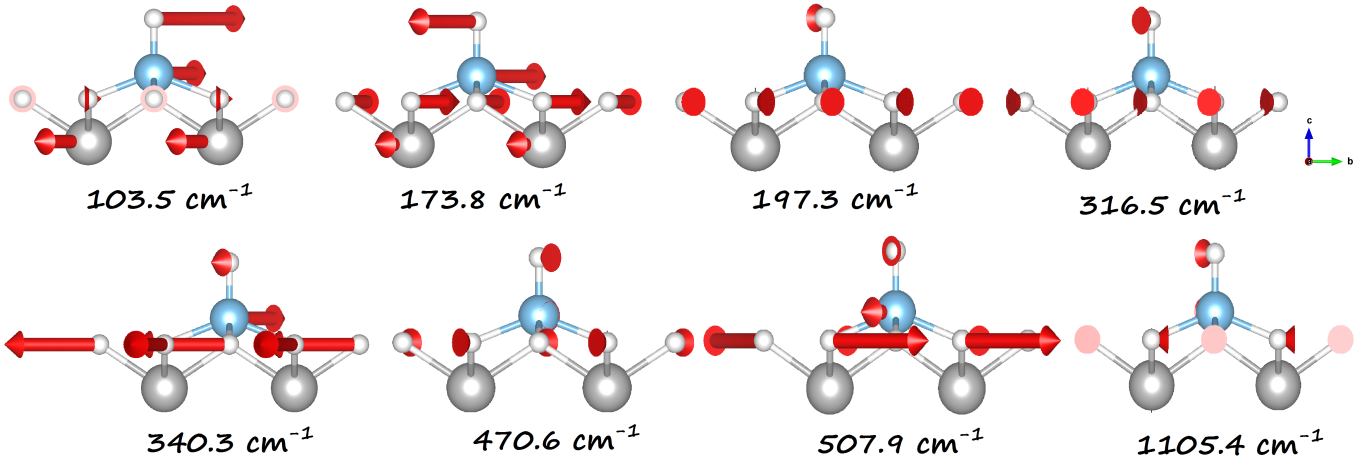


Fig. S2 (Color online) vibrational eigenvectors of the zone-centered acoustic phonon modes shown in the low dimensional $PbTiO_3$ structure. The light blue, white, and gray balls represent Ti, O, and Pb atoms, respectively

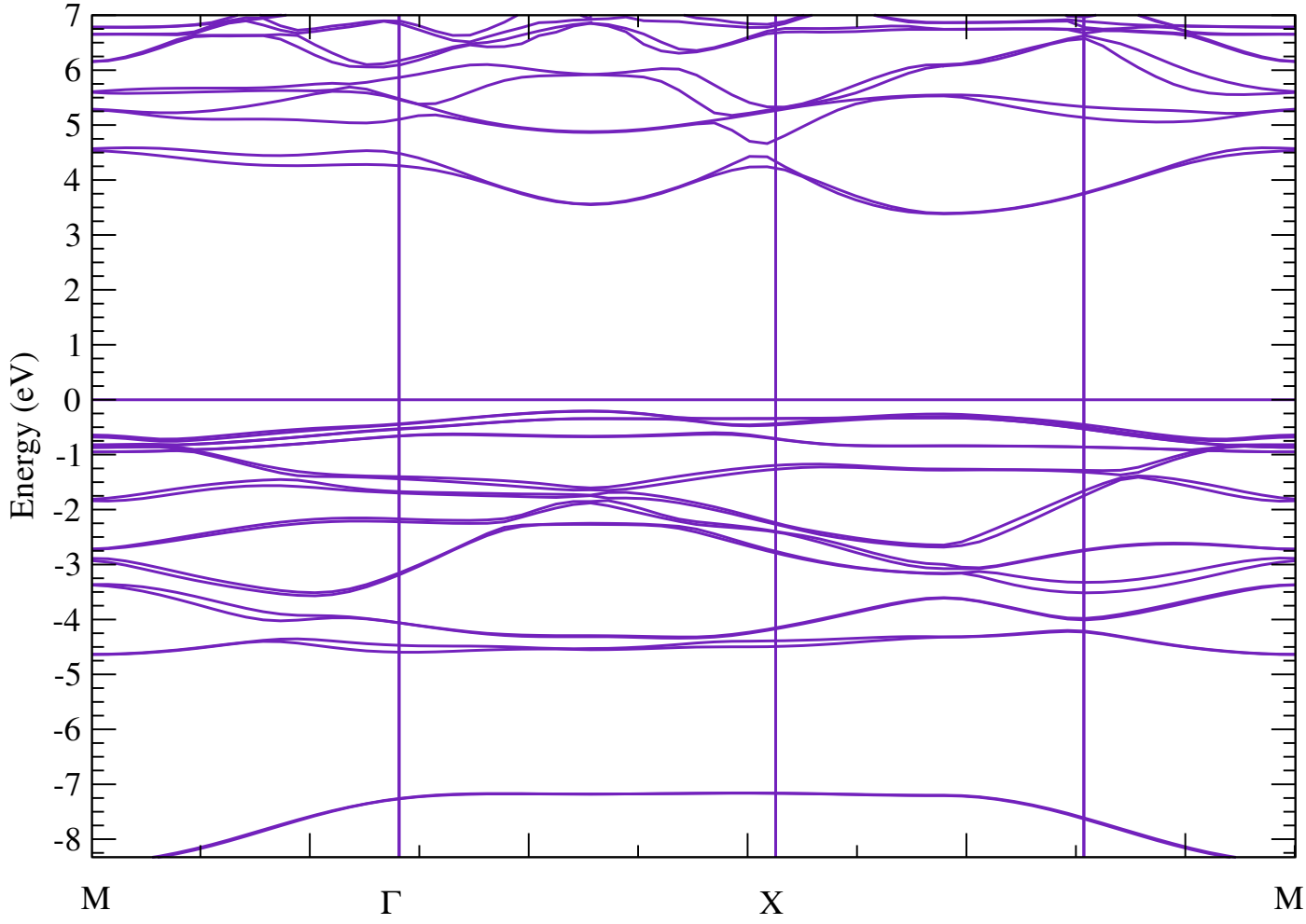


Fig. S3 (Color online) band structure plot for pristine low dimensional $PbTiO_3$ structure at DFT + $U$ + SOC level

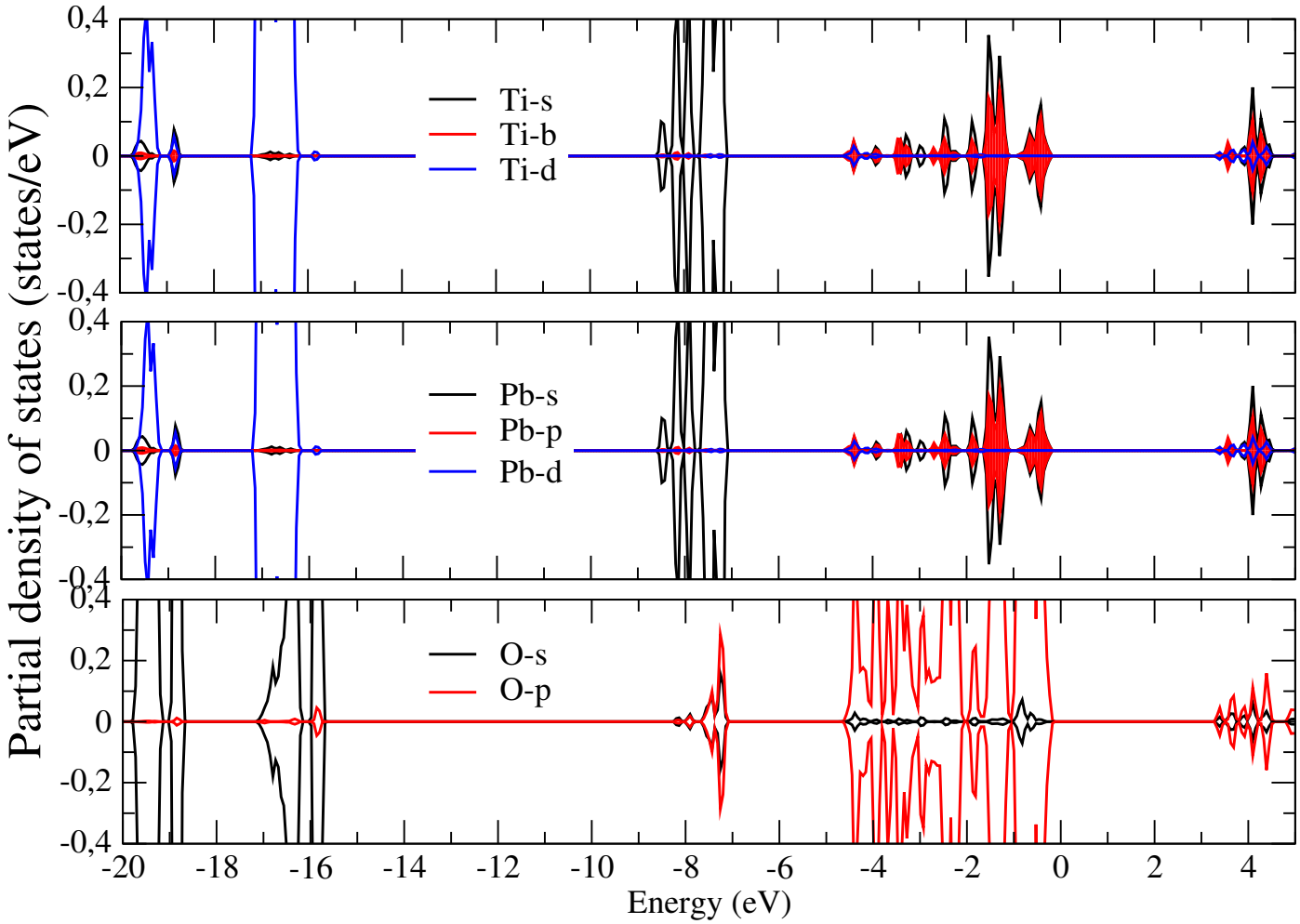


Fig. S4 (Color online) Projected densities of states (PDOS) of pristine low dimensional $PbTiO_3$ structure DFT + $U$ level.