Supporting Information
First-Principles Simulation of Monolayer Hydrogen Passivated $Bi_2O_2S_2$-Metal Interfaces

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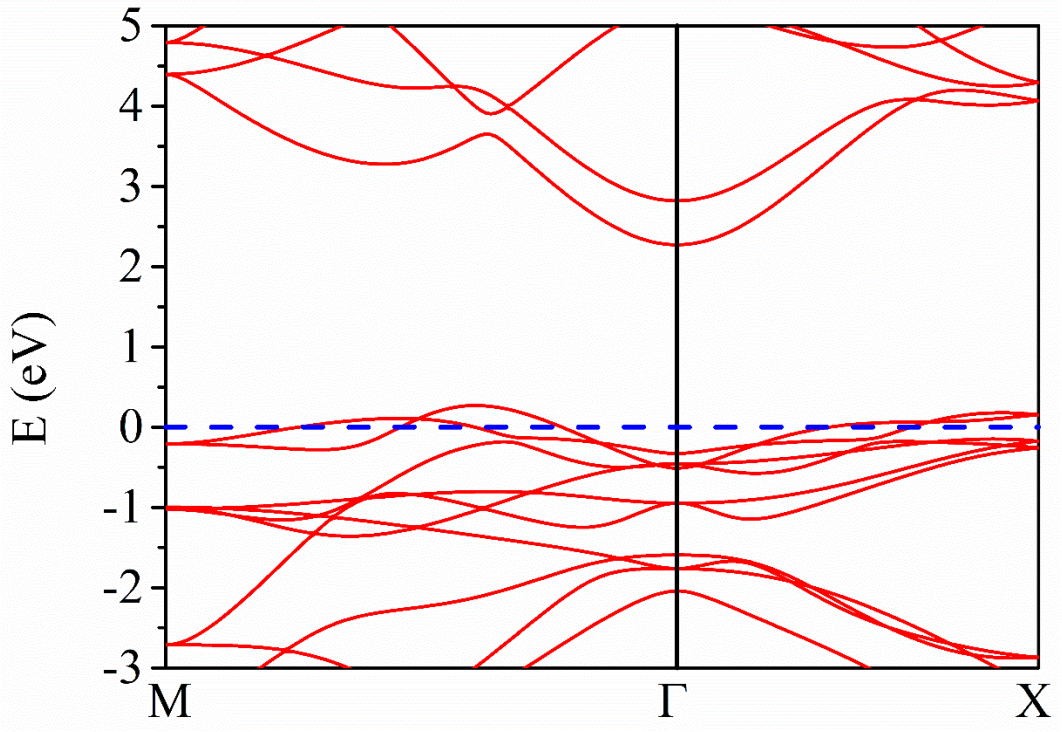

Figure S1. Band structure of ML $Bi_2O_2S_2$ without hydrogen passivation.

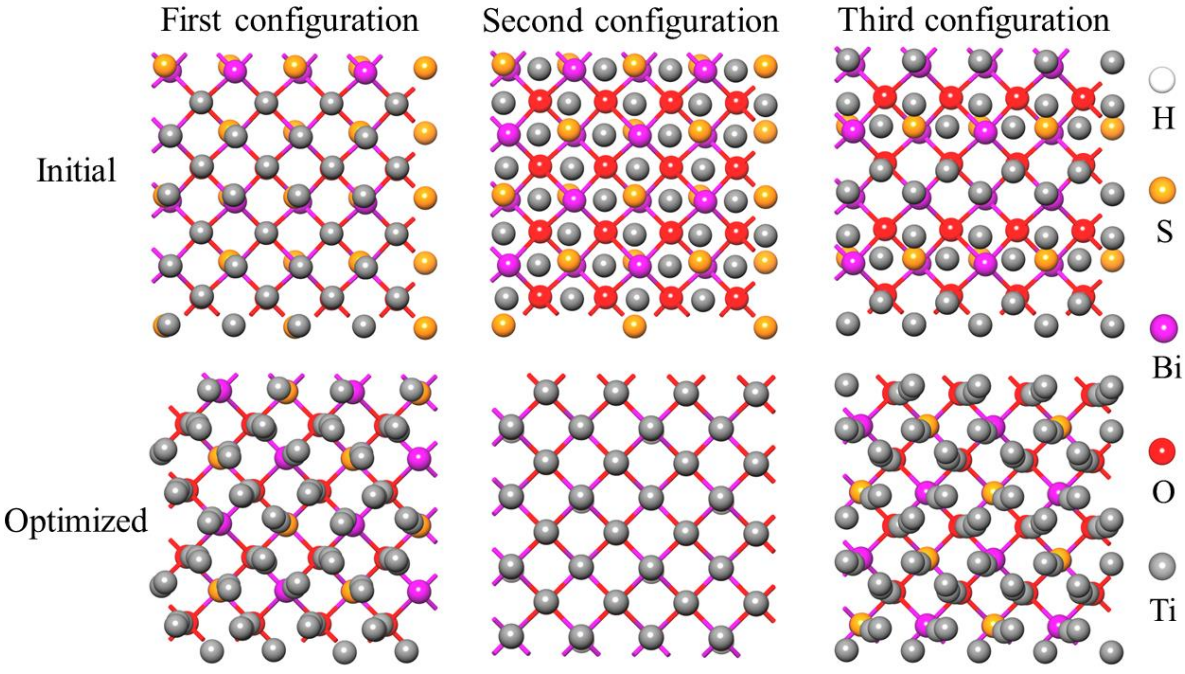

Figure S2. Three kinds of interfacial stacking configurations for Ti electrode. The first line displays the three initial configurations. The second line displays the three configurations after optimization. The corresponding atoms are shown on the right.

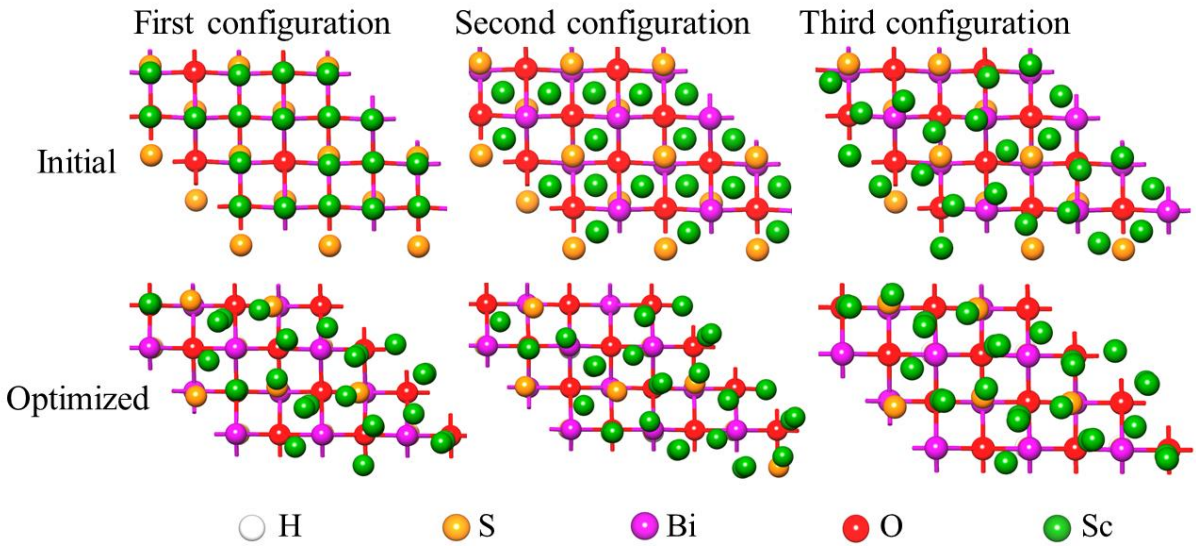

Figure S3. Three kinds of interfacial stacking configurations for Sc electrode. The first line displays the three initial configurations. The second line displays the three configurations after optimization. The corresponding atoms are shown on the bottom.

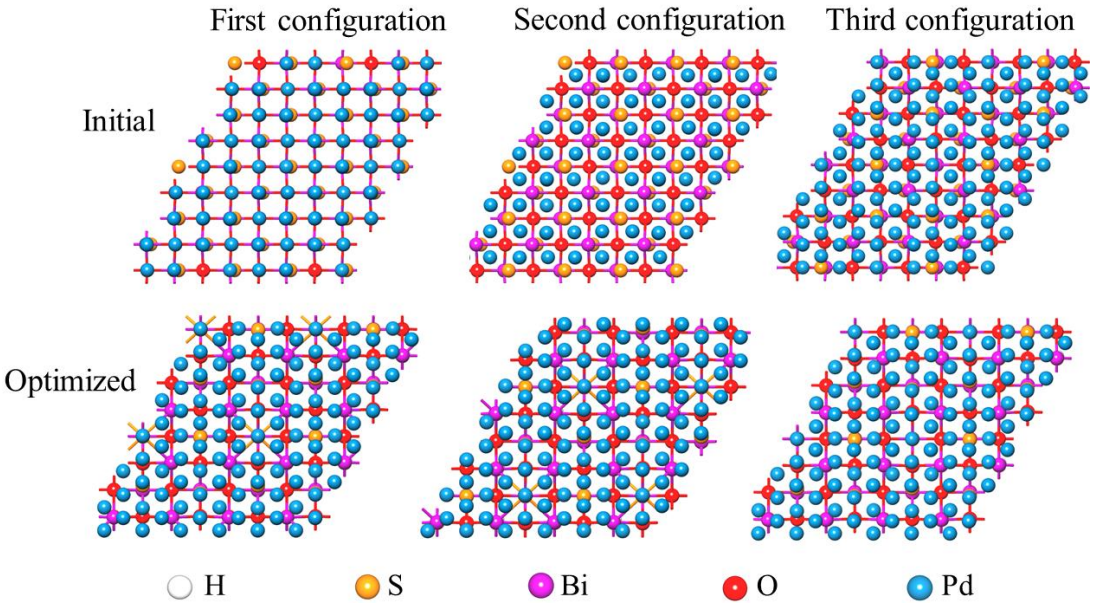

Figure S4. Three kinds of interfacial stacking configurations for Pd electrode. The first line displays the three initial configurations. The second line displays the three configurations after optimization. The corresponding atoms are shown on the bottom.

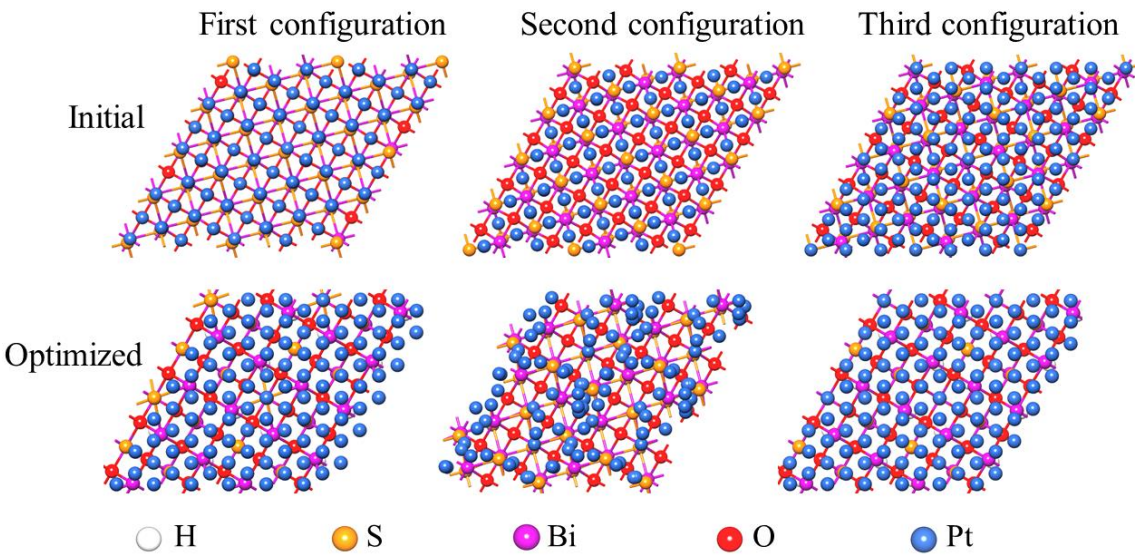

Figure S5. Three kinds of interfacial stacking configurations for Pt electrode. The first line displays the three initial configurations. The second line displays the three configurations after optimization. The corresponding atoms are shown on the bottom.