Electronic Supplementary Material for PCCP

Electronic Supporting Information

Density functional theory calculations for the hydrogen evolution reaction in an electrochemical double layer on the Pt(111) electrode

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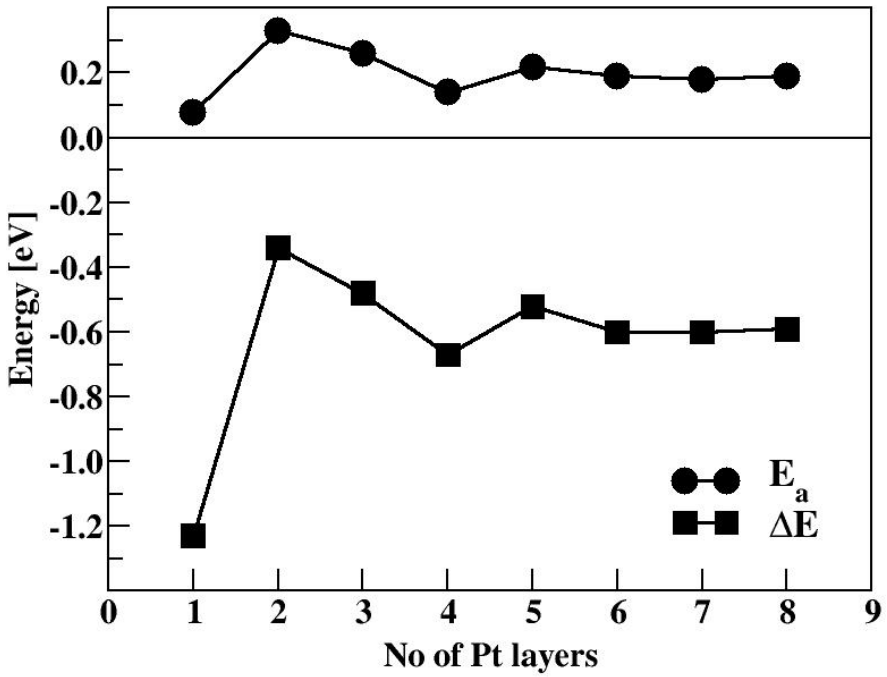

Figure S1: *The variation of the activation energy (circles) and the reaction energy (squares) with number of Pt layers used for the Density Functional Theory calculations. These tests were made by calculating the IS, TS and FS for the Heyrovsky reaction ($H^+ + e^- + H_{ad} \rightarrow H_2$) with 1-8 Pt layers. The energy values have converged completely using 6 Pt layers in the model system. In the present study we have chosen 3 Pt layers to save computational time. The difference between the 3 Pt layers and the 8 Pt layers test cases is very small, 0.07 eV for the activation energy and 0.11 eV for the reaction energy.*

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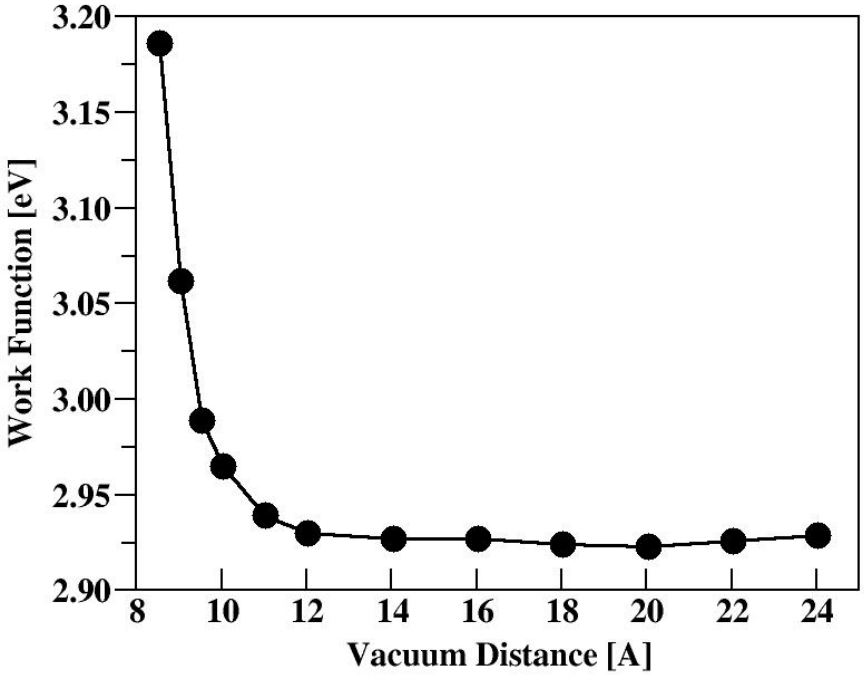

Figure S2: *The variation of the work function with increasing vacuum distance between the repeated slabs. The test case is the IS for the Heyrovsky reaction ($H^+ + e^- + H_{ad}$ -> H_2). The work function has completely converged with 12 Å of vacuum. In the present study we use 10 Å of vacuum for this system. The difference in the work function obtained by using 10 Å or 12 Å of vacuum is very small, or 0.035 eV, not affecting the trends observed in the study.*