Supplementary Information

for

Density Functional Theory Study of Thermodynamic and Kinetic Isotope Effects of H\textsubscript{2}/D\textsubscript{2} Dissociative Adsorption on Transition Metals

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\textbf{Figure S1.} Arrhenius plots for the thermodynamic isotope effects of H\textsubscript{2} and D\textsubscript{2} dissociative adsorption on the stable top sites of close-packed surfaces of transition metals.
Figure S2. Arrhenius plots for the thermodynamic isotope effects of H$_2$ and D$_2$ dissociative adsorption on the stable hcp sites of close-packed surfaces of transition metals.

Figure S3. Arrhenius plots for the thermodynamic isotope effects of H$_2$ and D$_2$ dissociative adsorption on the stable fcc sites of close-packed surfaces of transition metals.
Figure S4. Arrhenius plots for the thermodynamic isotope effects of $\text{H}_2$ and $\text{D}_2$ dissociative adsorption on the stable top sites of (100) surfaces of transition metals.

Figure S5. Arrhenius plots for the thermodynamic isotope effects of $\text{H}_2$ and $\text{D}_2$ dissociative adsorption on the stable bridge sites of (100) surfaces of transition metals.
Figure S6. Arrhenius plots for the thermodynamic isotope effects of H$_2$ and D$_2$ dissociative adsorption on the stable hollow sites of (100) surfaces of transition metals.

Figure S7. Arrhenius plots for the thermodynamic isotope effects of H$_2$ and D$_2$ dissociative adsorption on the stable top_a sites of (211) surfaces of transition metals.
Figure S8. Arrhenius plots for the thermodynamic isotope effects of $\text{H}_2$ and $\text{D}_2$ dissociative adsorption on the stable top$_b$ sites of (211) surfaces of transition metals.

Figure S9. Arrhenius plots for the thermodynamic isotope effects of $\text{H}_2$ and $\text{D}_2$ dissociative adsorption on the stable top$_c$ sites of (211) surfaces of transition metals.
Figure S10. Arrhenius plots for the thermodynamic isotope effects of H\textsubscript{2} and D\textsubscript{2} dissociative adsorption on the stable bridge\_a sites of (211) surfaces of transition metals.

Figure S11. Arrhenius plots for the thermodynamic isotope effects of H\textsubscript{2} and D\textsubscript{2} dissociative adsorption on the stable bridge\_bc sites of (211) surfaces of transition metals.
**Figure S12.** Arrhenius plots for the thermodynamic isotope effects of H$_2$ and D$_2$ dissociative adsorption on the stable bridge_ca sites of (211) surfaces of transition metals.

**Figure S13.** Arrhenius plots for the thermodynamic isotope effects of H$_2$ and D$_2$ dissociative adsorption on the stable hollow_a1 sites of (211) surfaces of transition metals.
**Figure S14.** Arrhenius plots for the thermodynamic isotope effects of H$_2$ and D$_2$ dissociative adsorption on the stable hollow$_{a2}$ sites of (211) surfaces of transition metals.

**Figure S15.** Arrhenius plots for the thermodynamic isotope effects of H$_2$ and D$_2$ dissociative adsorption on the stable hollow$_{b1}$ sites of (211) surfaces of transition metals.
Figure S16. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable hollow_b2 sites of (211) surfaces of transition metals.

Figure S17. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable hollow_c1 sites of (211) surfaces of transition metals.
**Figure S18.** Arrhenius plots for the thermodynamic isotope effects of H\(_2\) and D\(_2\) dissociative adsorption on the stable hollow\_c2 sites of (211) surfaces of transition metals.