

Supplementary Information

for

Density Functional Theory Study of Thermodynamic and Kinetic Isotope Effects of H₂/D₂ Dissociative Adsorption on Transition Metals

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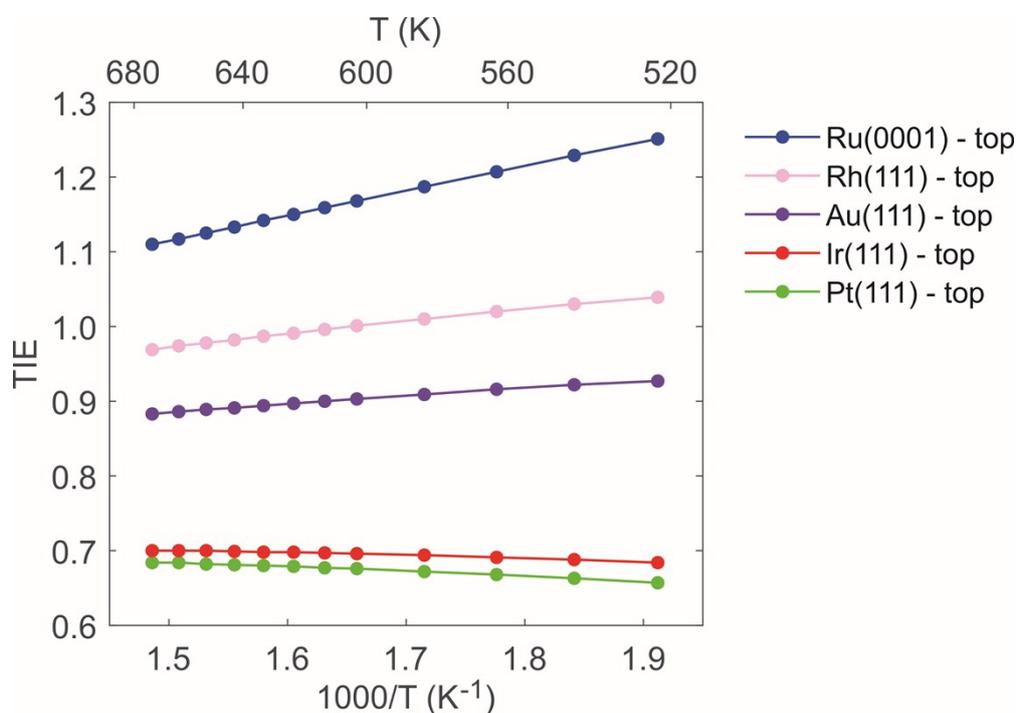


Figure S1. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable top sites of close-packed surfaces of transition metals.

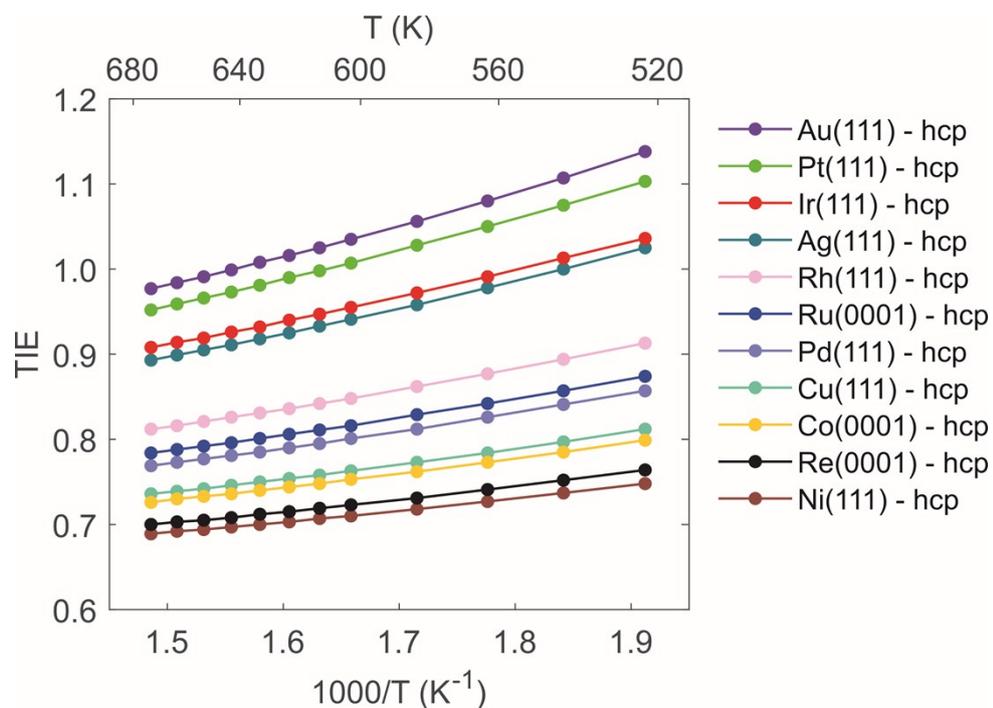


Figure S2. Arrhenius plots for the thermodynamic isotope effects of H_2 and D_2 dissociative adsorption on the stable hcp sites of close-packed surfaces of transition metals.

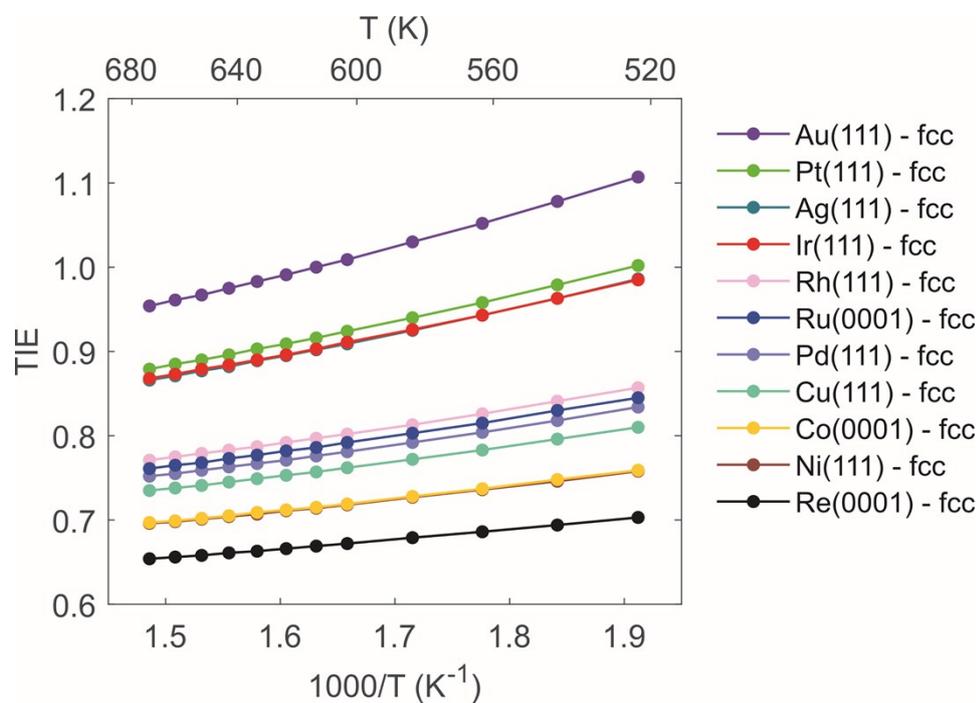


Figure S3. Arrhenius plots for the thermodynamic isotope effects of H_2 and D_2 dissociative adsorption on the stable fcc sites of close-packed surfaces of transition metals.

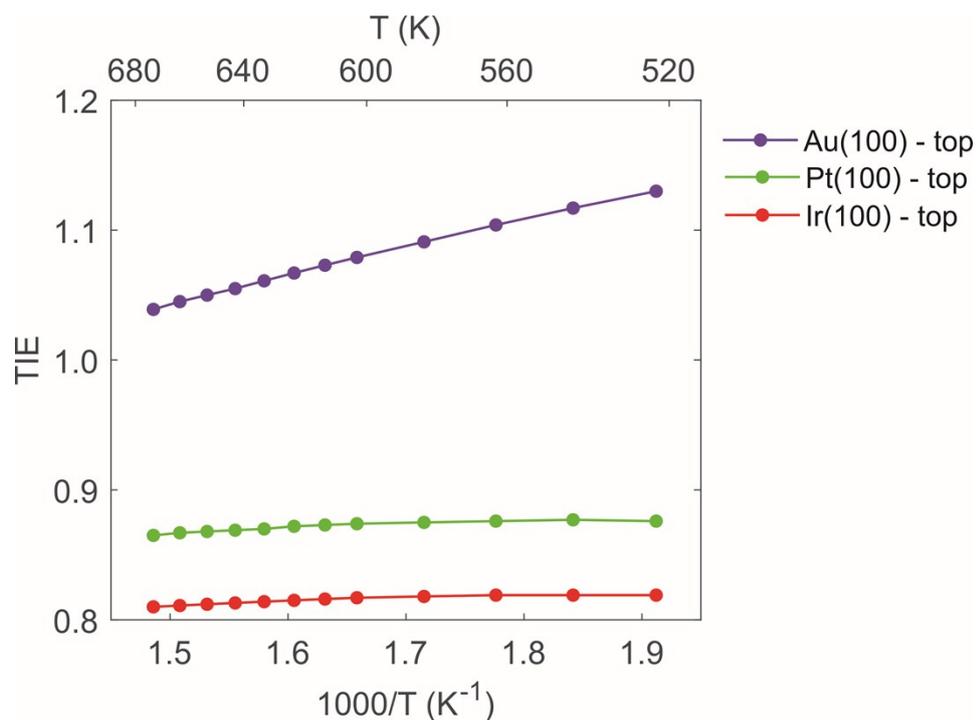


Figure S4. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable top sites of (100) surfaces of transition metals.

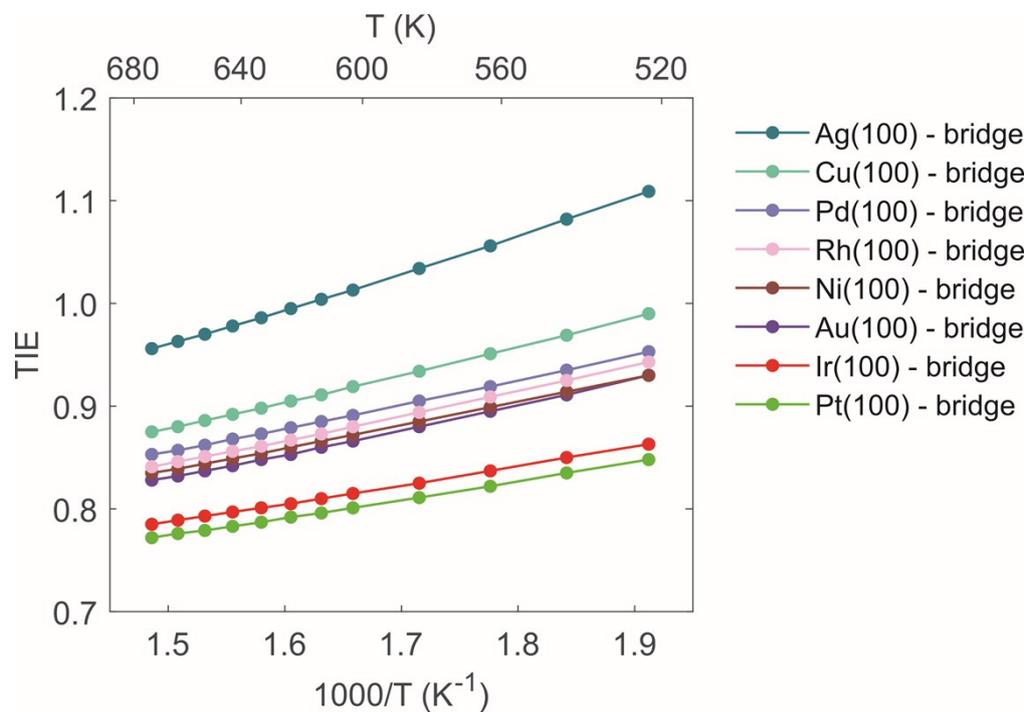


Figure S5. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable bridge sites of (100) surfaces of transition metals.

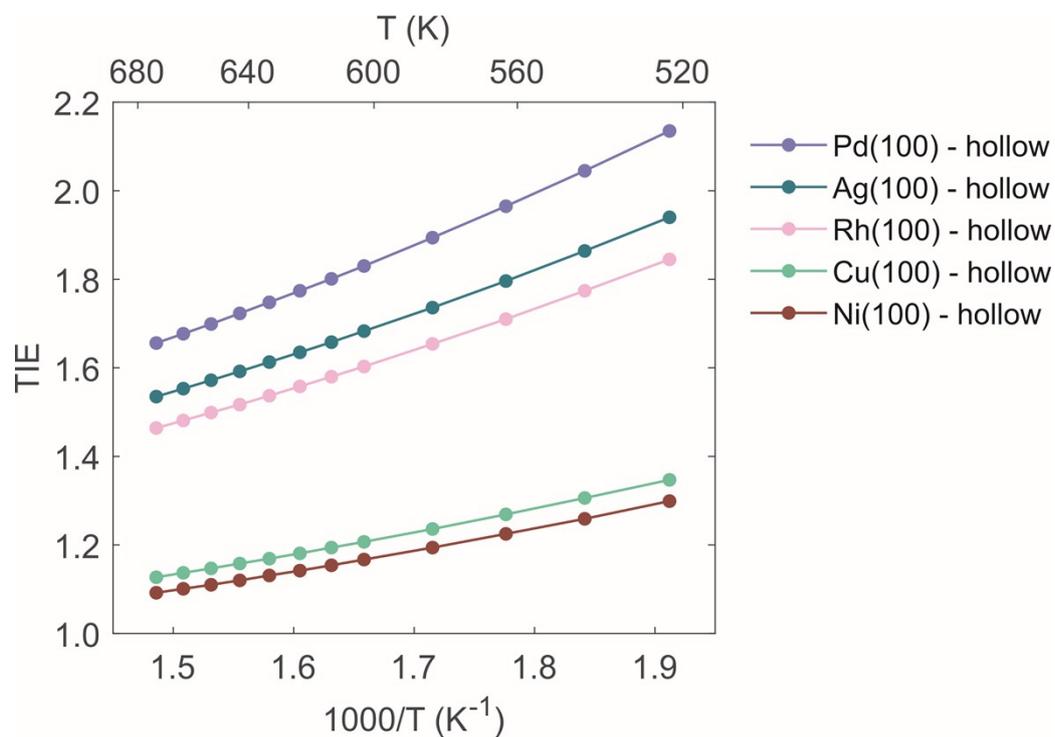


Figure S6. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable hollow sites of (100) surfaces of transition metals.

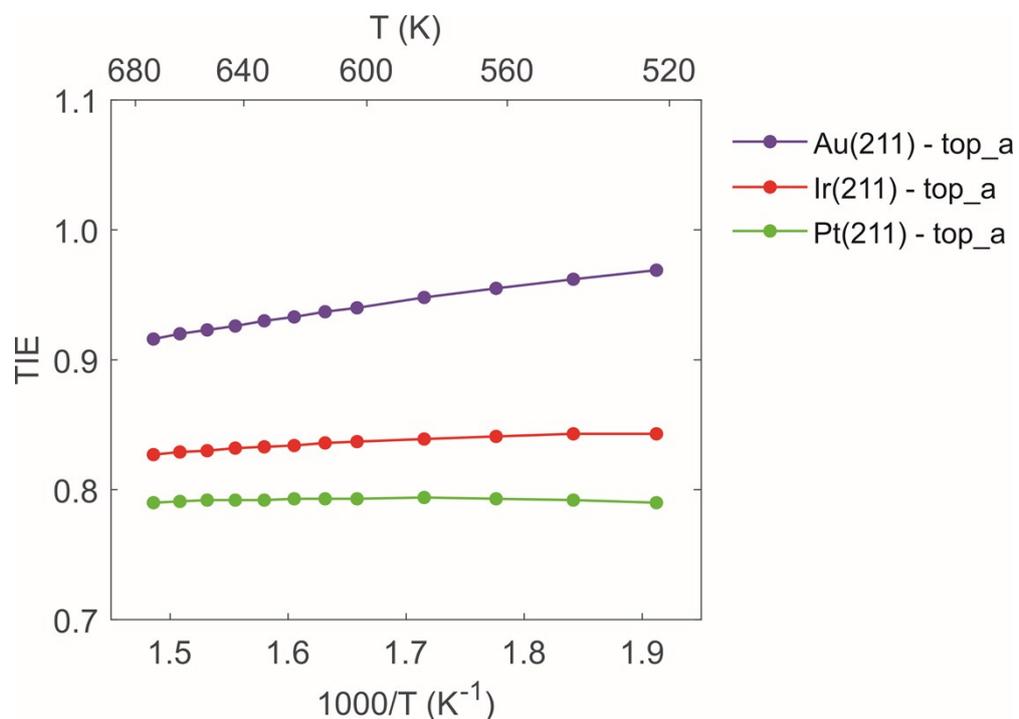


Figure S7. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable top_a sites of (211) surfaces of transition metals.

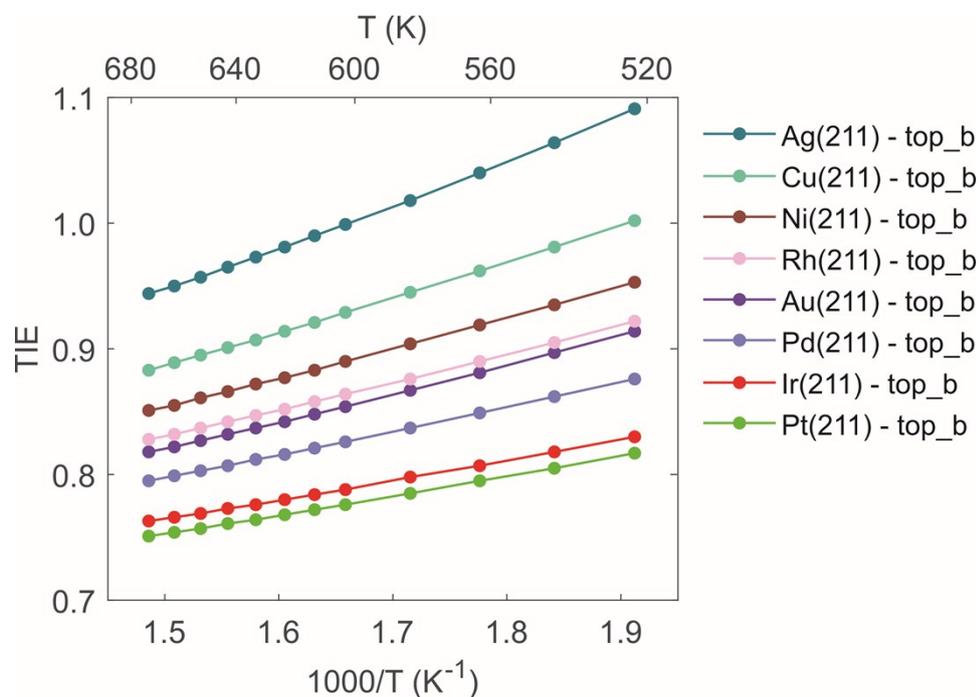


Figure S8. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable top_b sites of (211) surfaces of transition metals.

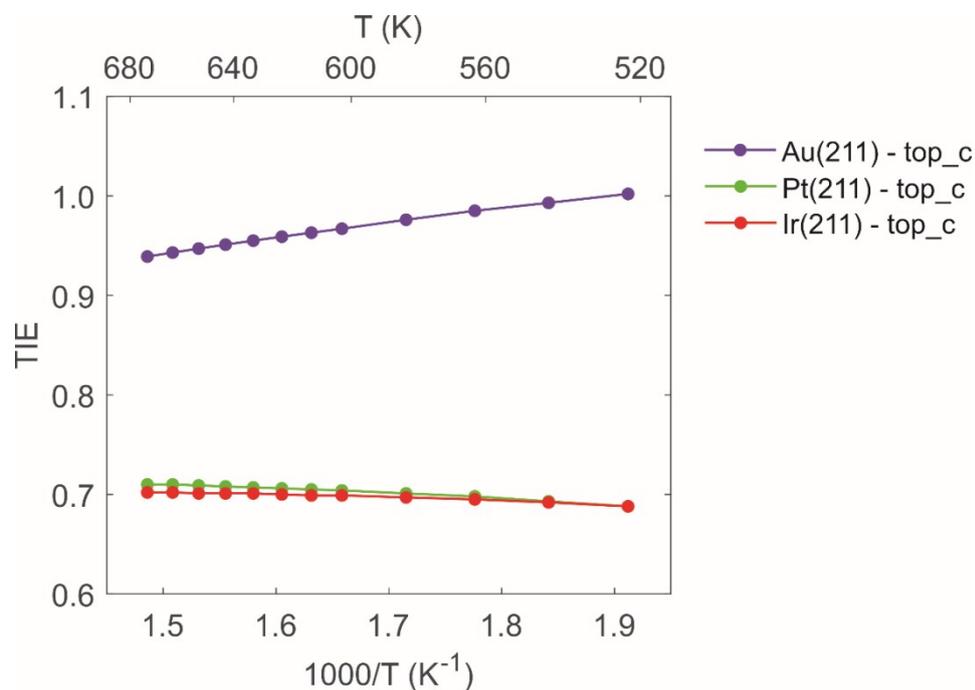


Figure S9. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable top_c sites of (211) surfaces of transition metals.

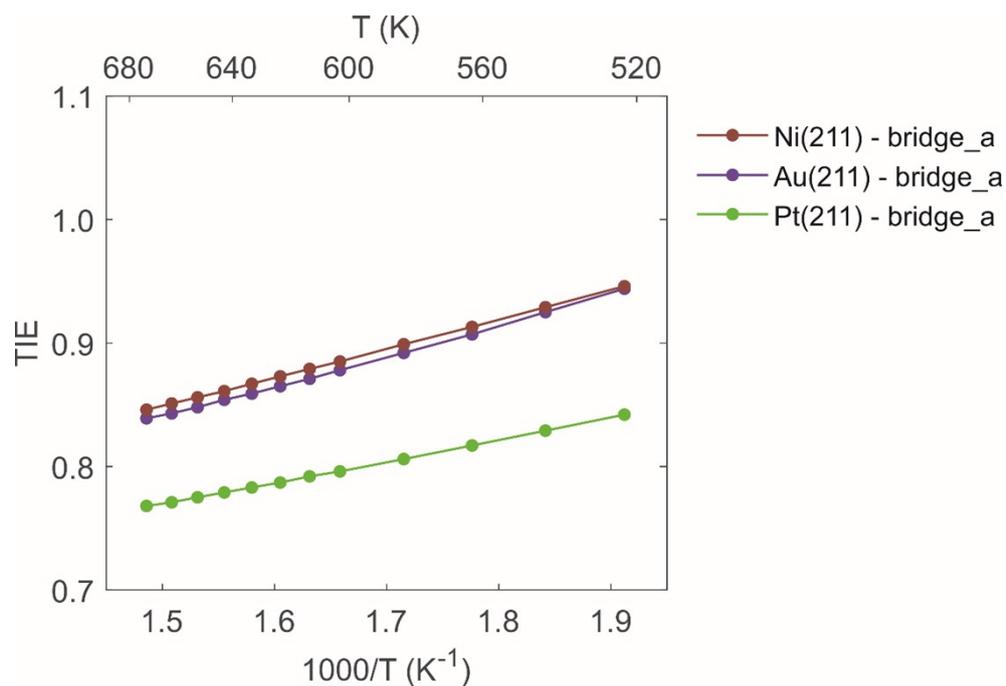


Figure S10. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable bridge_a sites of (211) surfaces of transition metals.

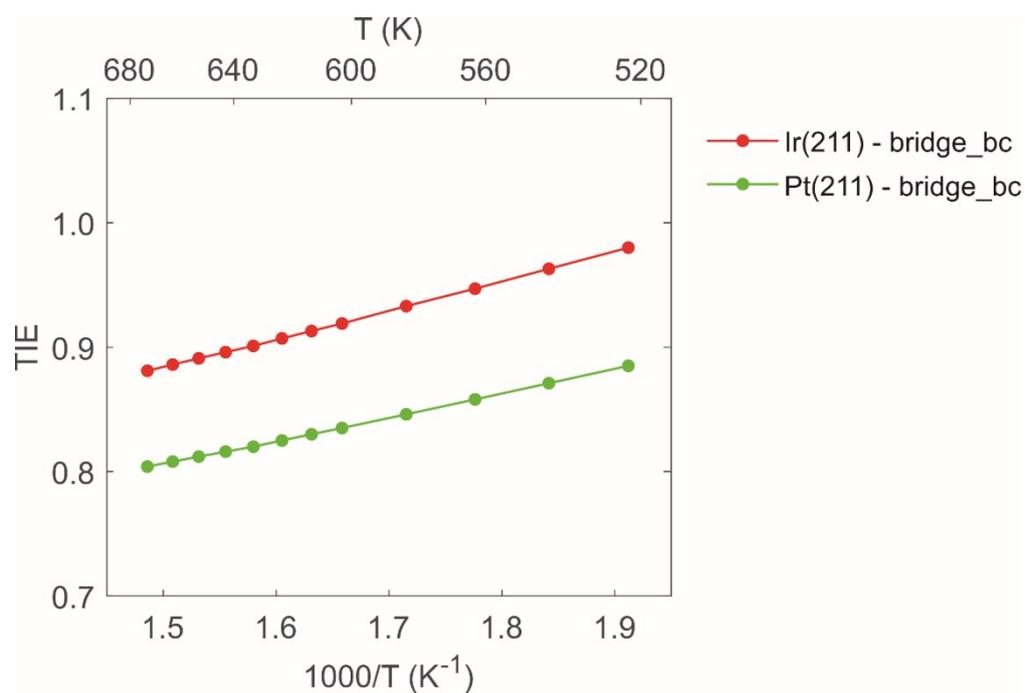


Figure S11. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable bridge_bc sites of (211) surfaces of transition metals.

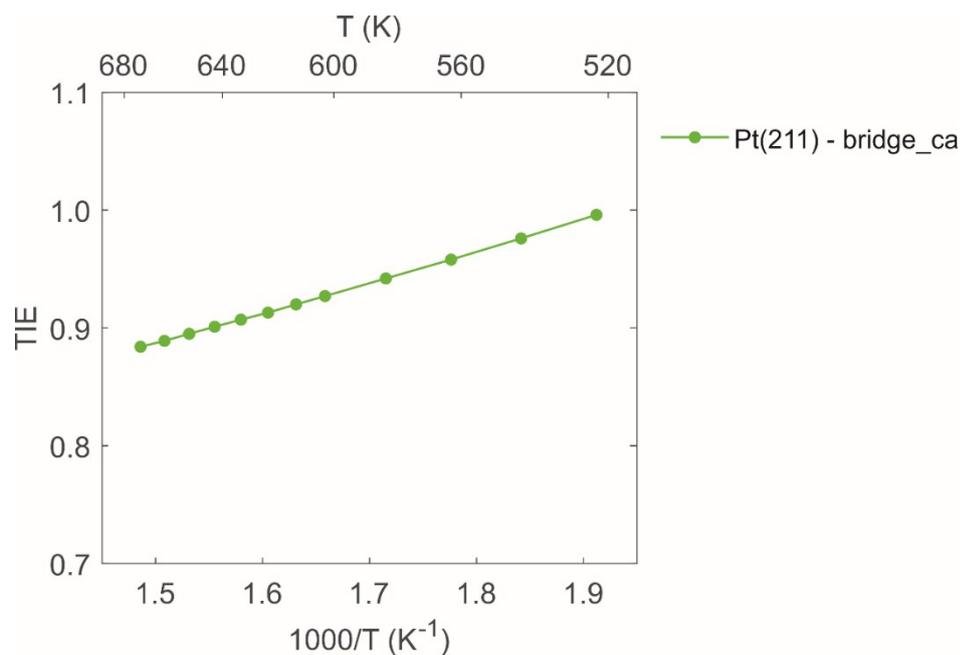


Figure S12. Arrhenius plots for the thermodynamic isotope effects of H_2 and D_2 dissociative adsorption on the stable bridge_ca sites of (211) surfaces of transition metals.

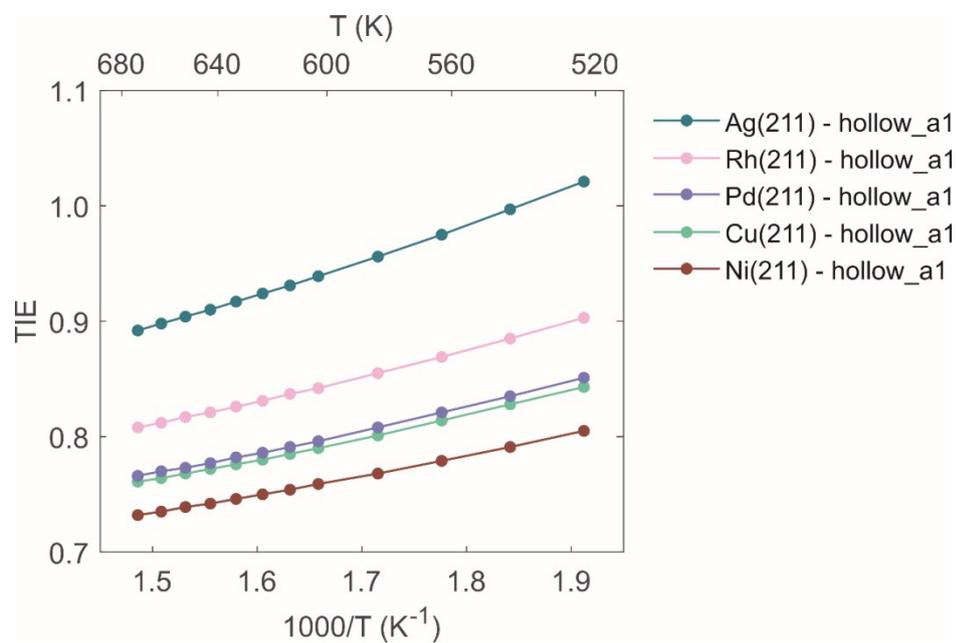


Figure S13. Arrhenius plots for the thermodynamic isotope effects of H_2 and D_2 dissociative adsorption on the stable hollow_a1 sites of (211) surfaces of transition metals.

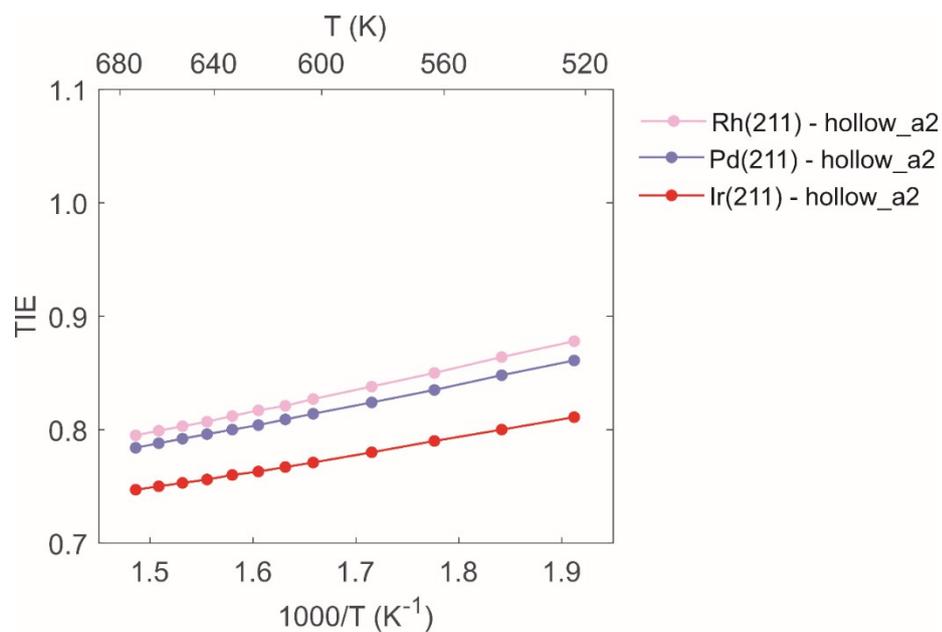


Figure S14. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable hollow_a2 sites of (211) surfaces of transition metals.

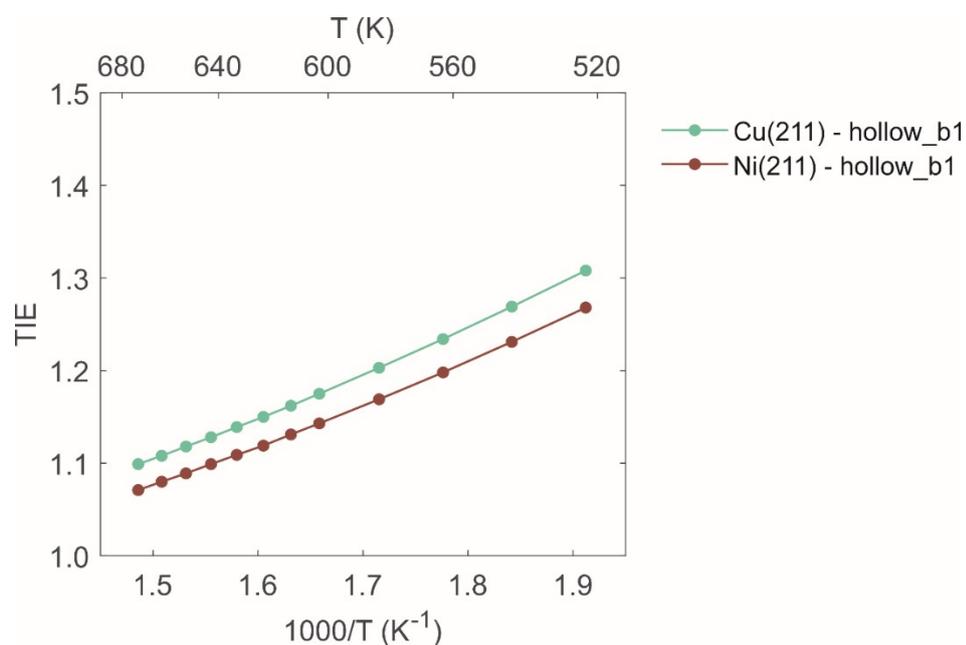


Figure S15. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable hollow_b1 sites of (211) surfaces of transition metals.

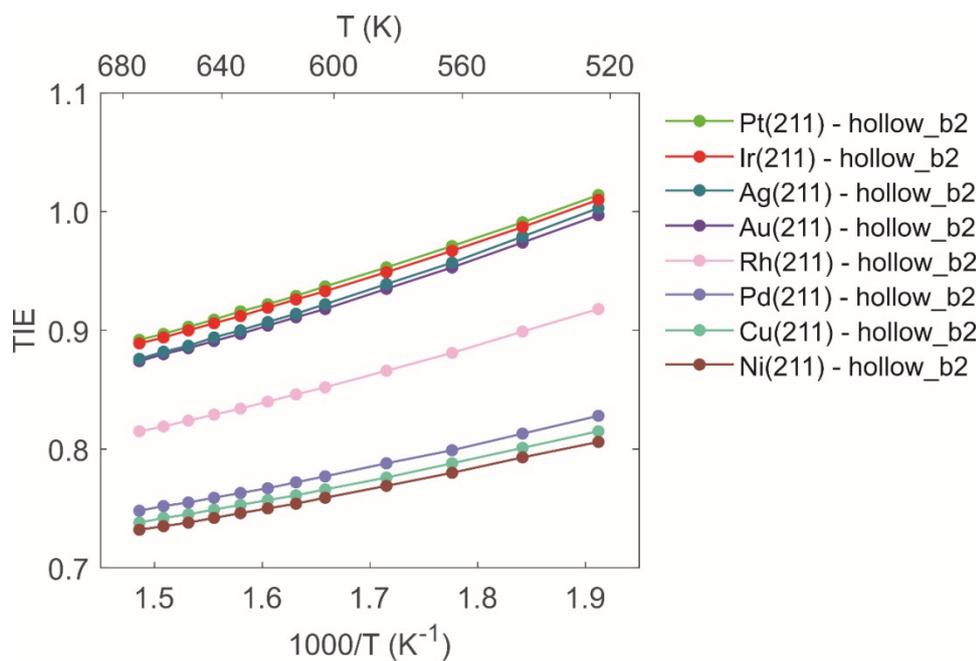


Figure S16. Arrhenius plots for the thermodynamic isotope effects of H_2 and D_2 dissociative adsorption on the stable hollow_b2 sites of (211) surfaces of transition metals.

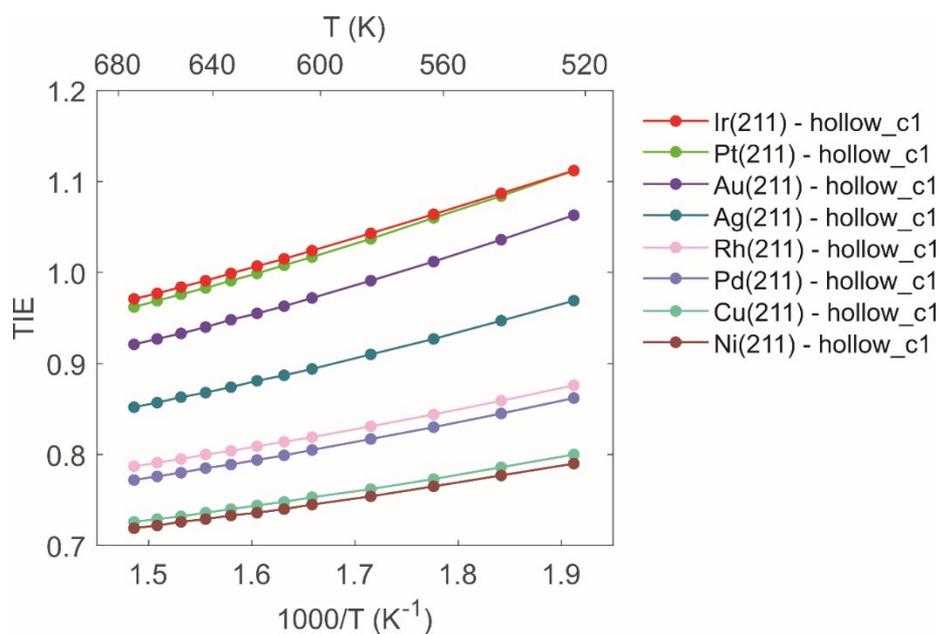


Figure S17. Arrhenius plots for the thermodynamic isotope effects of H_2 and D_2 dissociative adsorption on the stable hollow_c1 sites of (211) surfaces of transition metals.

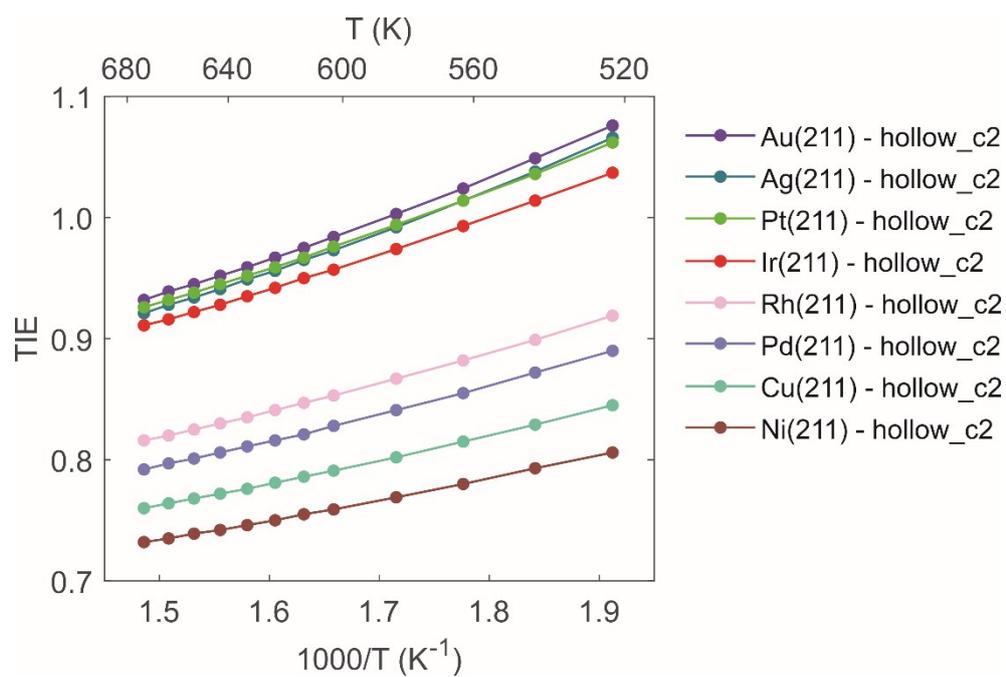


Figure S18. Arrhenius plots for the thermodynamic isotope effects of H₂ and D₂ dissociative adsorption on the stable hollow_c2 sites of (211) surfaces of transition metals.