Adsorption of Thiophene on Transition Metal Surfaces with the Inclusion of van der Waals Effects

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Highlights

- Density functional theory (DFT) with and without the inclusion of van der Waals interactions was utilized to study the adsorption of thiophene on various transition metal (100) surfaces.
- Thiophene chemisorpes on Rh,Pt, and Pd (100) surfaces while physisorpes on Ag and Au (100) surfaces.
- Adsorption height is independent of functional and metal for thiophene on Pt, Pd, and Rh (100) surfaces.
- A net negative charge is transferred from the thiophene molecule to the surface except in the case of Rh(100).
- The inclusion of the van der Waals interaction can have a large effect on the results especially for the less reactive coinage metals.