Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information for: Chiral modification of platinum: Ab initio study of the effect of hydrogen coadsorption on stability and geometry of adsorbed cinchona alkaloids

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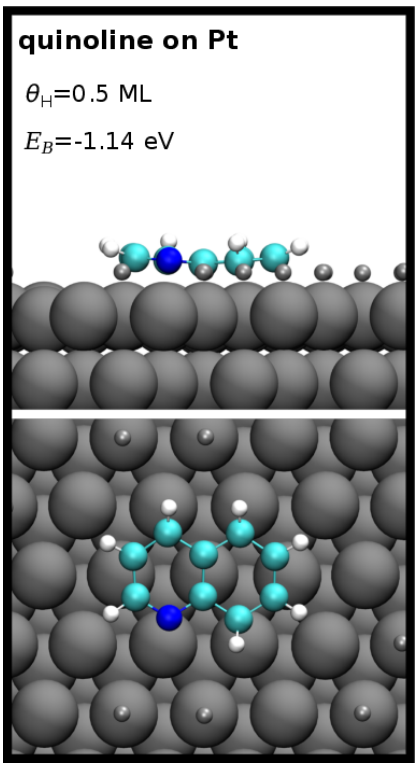

Figure 1: Stable configuration of quinoline on Pt(111)with θ_{H}=0.5 ML where the H atoms are segregated to leave enough active sites for the quinoline molecule to adsorb.

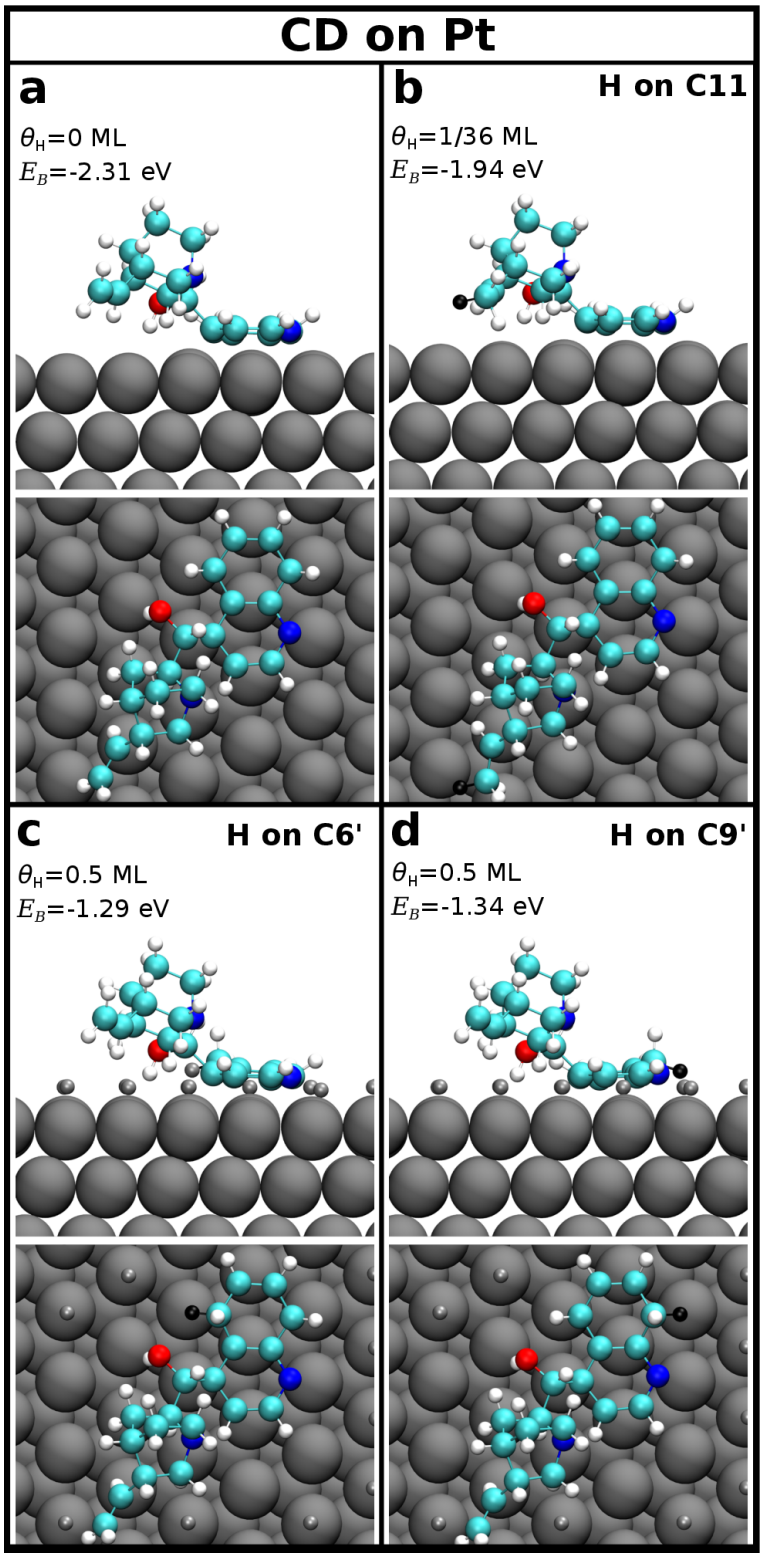

Figure 2: Stable configurations of CD on (a) clean Pt(111), (b) with θ_H=1/36 ML with the H atom transferred to the C11 atom and with θ_H=0.5 ML and (c) H transfer to the C6' atom and (d) to the C9' atom.

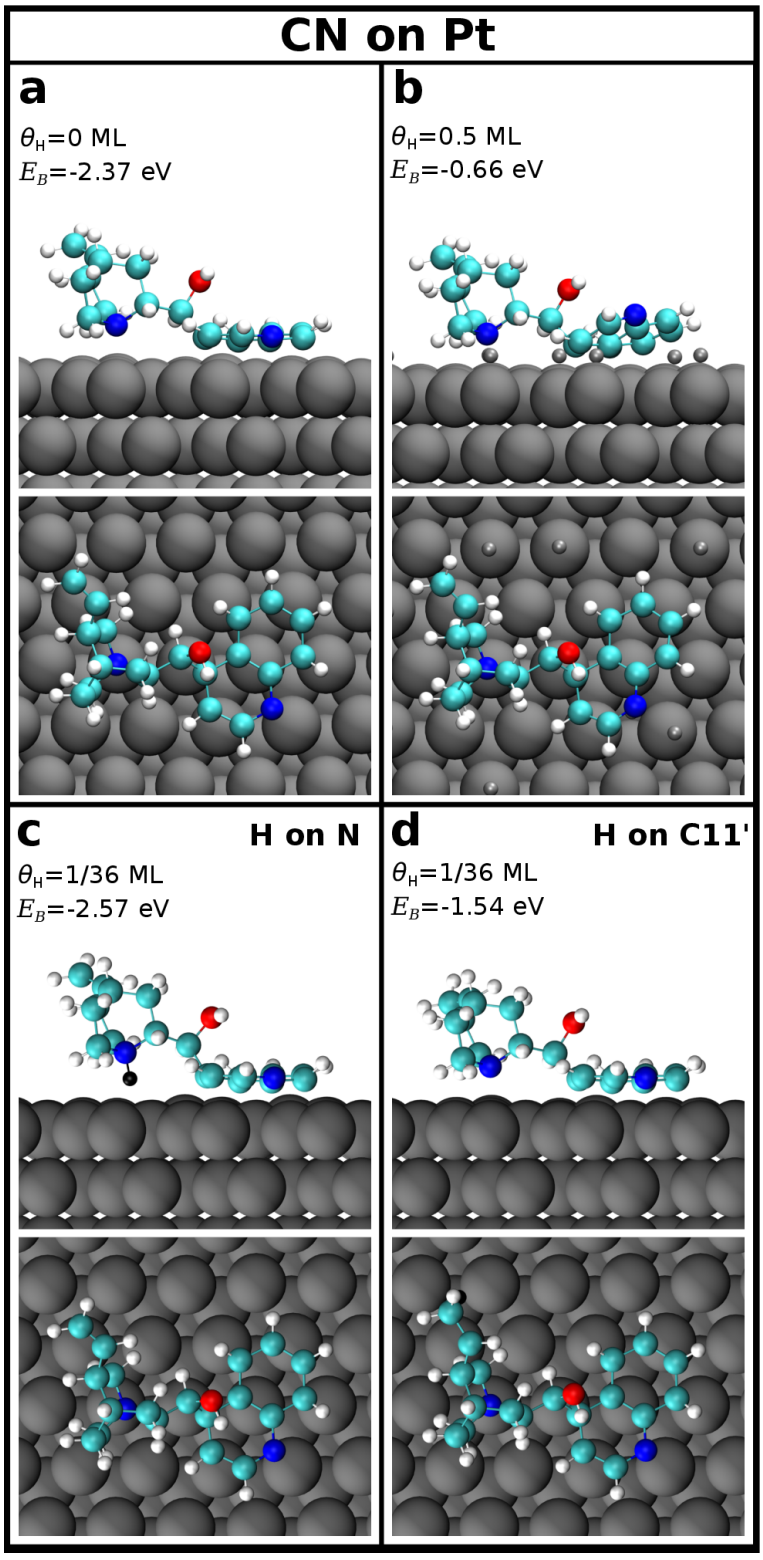

Figure 3: Stable configurations of CN on (a) clean Pt(111), (b) with θ_H=0.5 ML and H atoms adsorbed on active sites and with θ_H=1/36 ML and (c) H transfer to the N atom of the quinuclidine moiety and (d) the C11 atom.