Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Computational study of the adsorption and dissociation of phenol on Pt and Rh surfaces - *Supporting Information*

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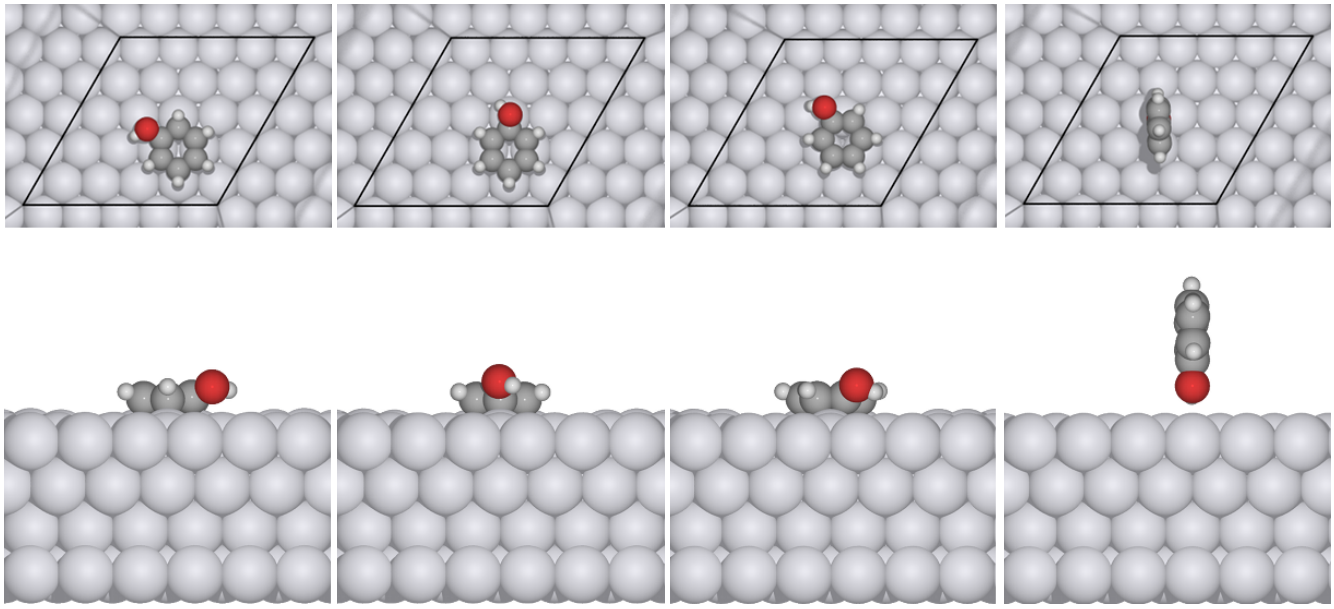
S.1 Phenol on Pt(111) and Rh(111)



(a) 2.233 eV (b) 2.106 eV (c) 1.918 eV (d) 1.089 eV

Figure S1 Top and side views of the most stable adsorption configurations with phenol adsorbed parallel (a-c) and vertically (d) on the Pt(111) surface, with corresponding binding energies indicated for each structure. The black lines in the top views indicate the surface unit cells used in the calculations.

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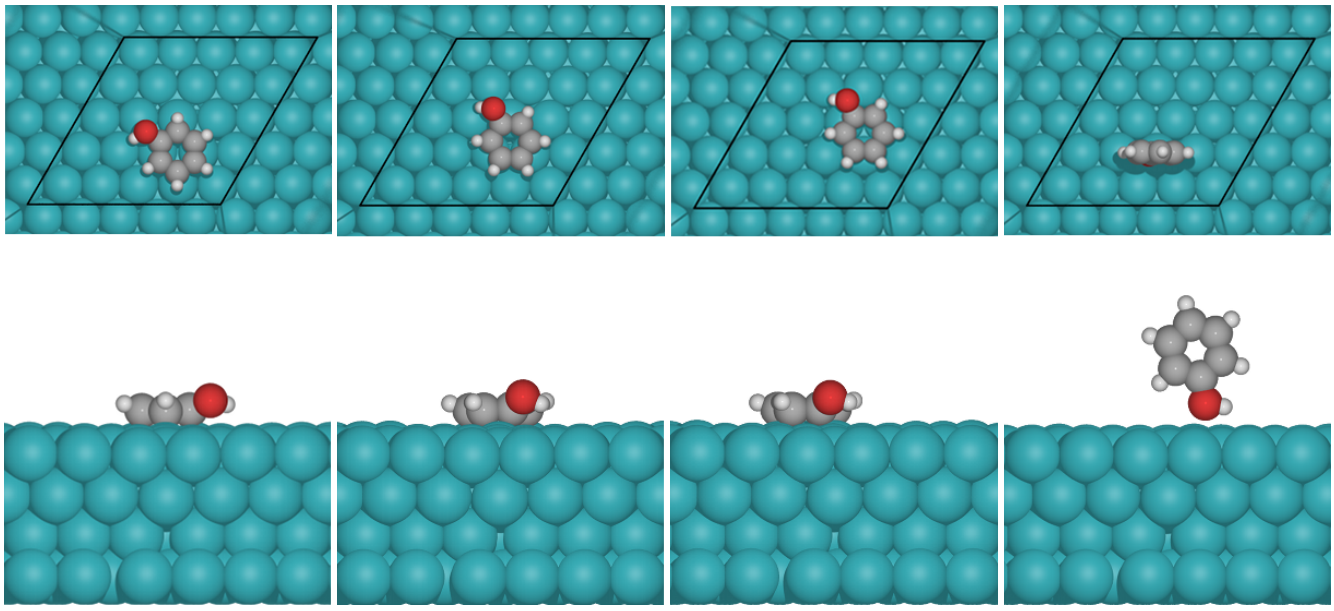
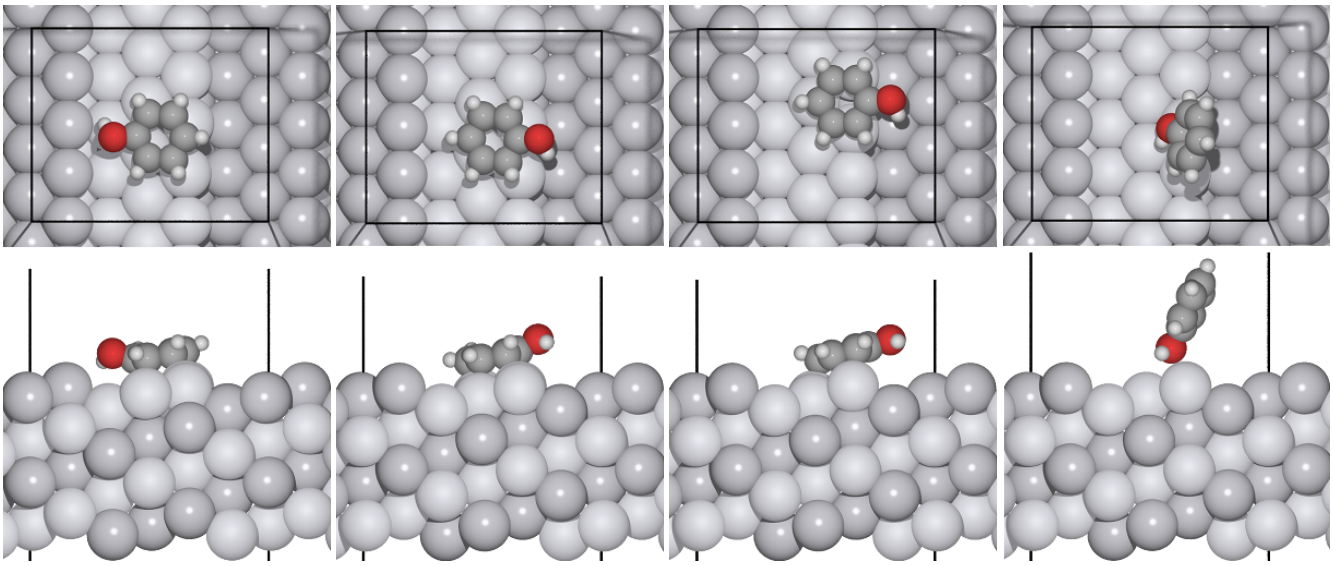


(a) 2.785 eV (b) 2.767 eV (c) 2.718 eV (d) 1.148 eV

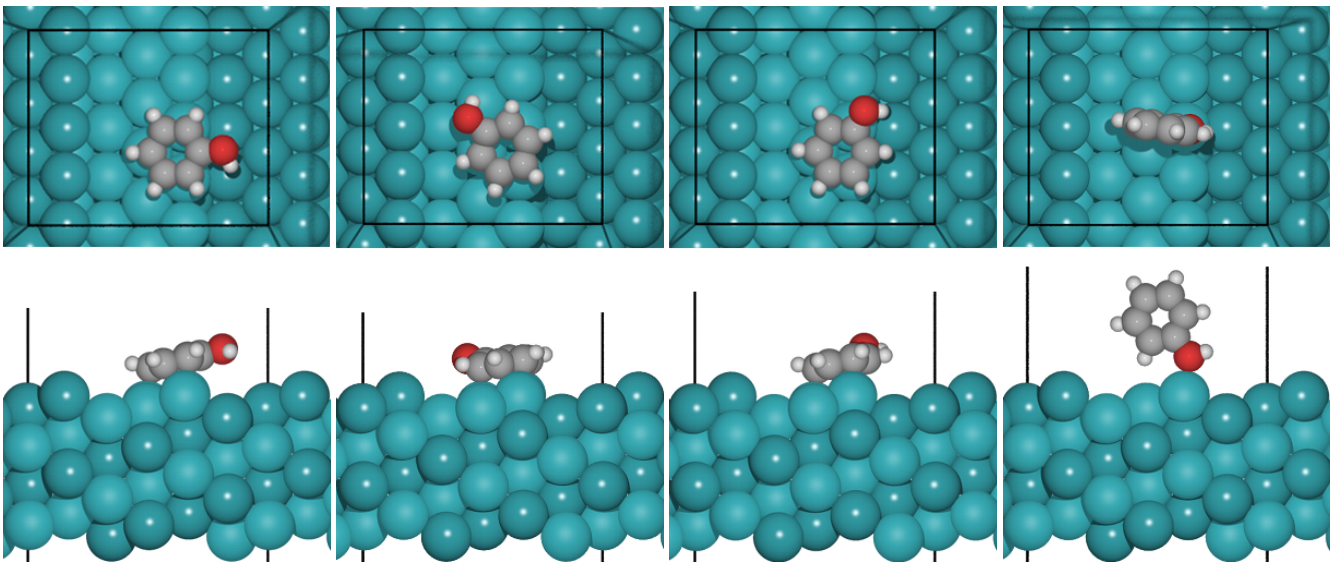
Figure S2 Top and side views of the most stable adsorption configurations with phenol adsorbed parallel (a-c) and vertically (d) on the Rh(111) surface, with corresponding binding energies indicated for each structure. The black lines in the top views indicate the surface unit cells used in the calculations.

S.2 Phenol on Pt(211) and Rh(211)



(a) 1.589 eV (b) 1.547 eV (c) 1.535 eV (d) 0.246 eV

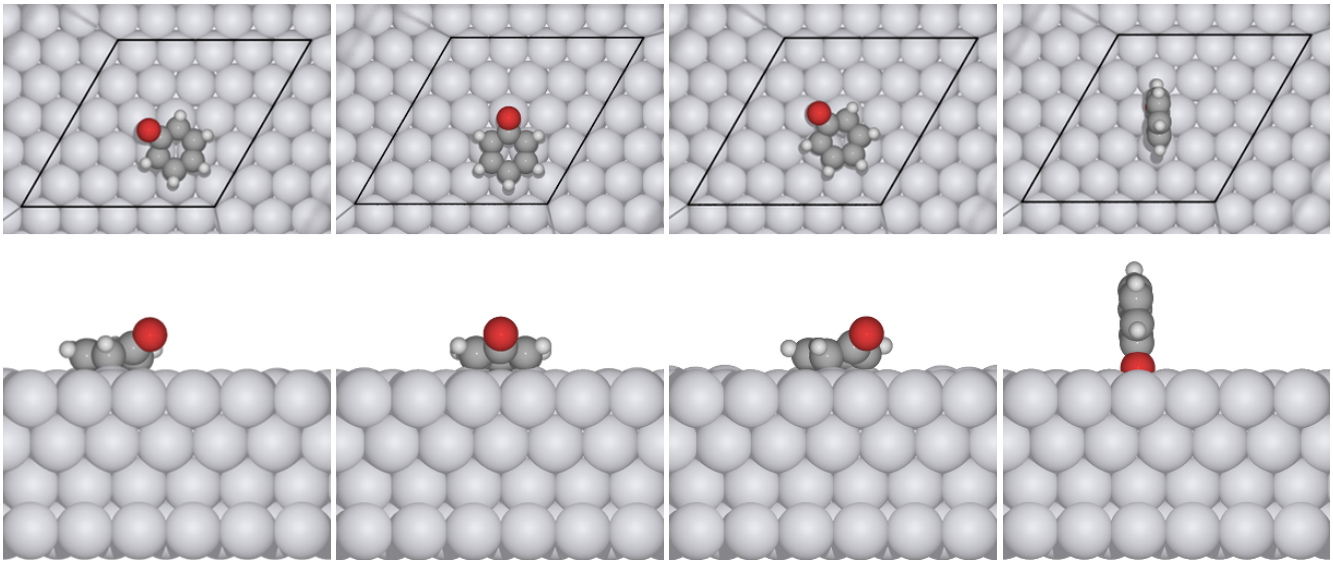
Figure S3 Top and side views of the most stable adsorption configurations with phenol adsorbed parallel on a terrace (a-c) and vertically (d) on the stepped Pt(211) surface, with corresponding binding energies indicated for each structure. The black lines indicate the surface unit cells used in the calculations.



(a) 1.785 eV (b) 1.738 eV (c) 1.550 eV (d) 0.364 eV

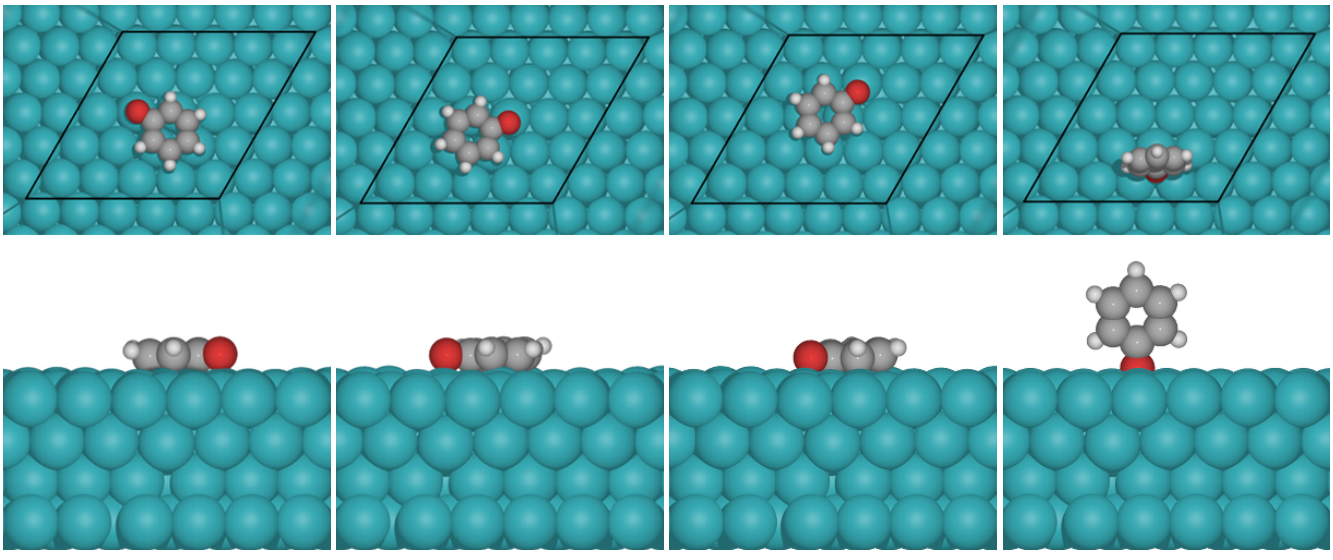
Figure S4 Top and side views of the most stable adsorption configurations with phenol adsorbed parallel on a terrace (a-c) and vertically (d) on the stepped Rh(211) surface, with corresponding binding energies indicated for each structure. The black lines indicate the surface unit cells used in the calculations.

S.3 Phenoxy on Pt(111) and Rh(111)



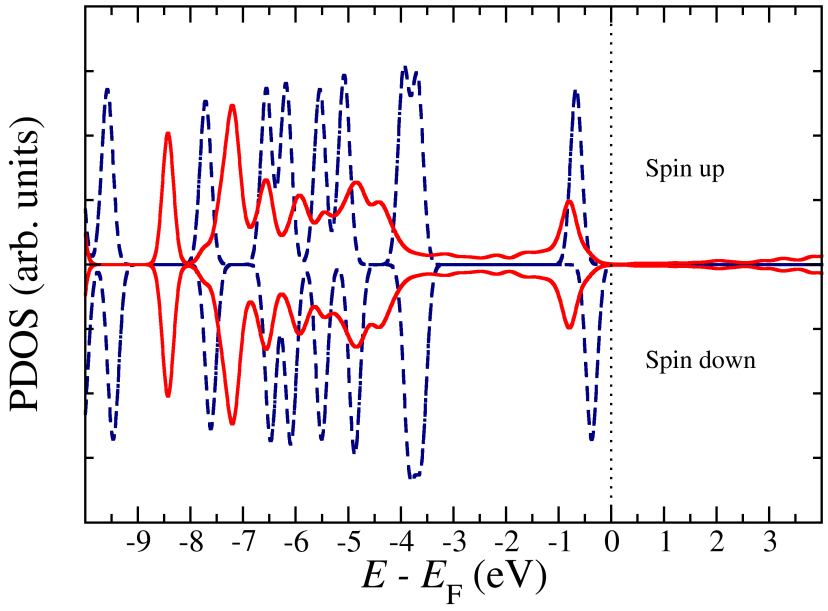
(a) 0.263 eV (b) 0.418 eV (c) 0.436 eV (d) 1.614 eV

Figure S5 Top and side views of the most stable adsorption configurations with phenoxy adsorbed parallel on a terrace (a-c) and vertically (d) on the Pt(111) surface, with corresponding reaction energy (with respect to the most stable adsorption site of phenol) indicated for each structure. The black lines in the top views indicate the surface unit cells used in the calculations.

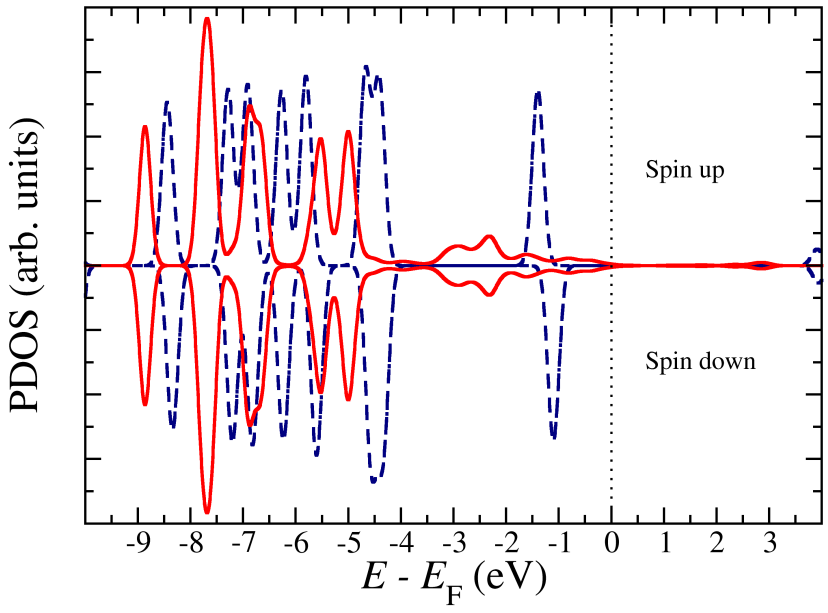


(a) -0.271 eV (b) -0.202 eV (c) -0.173 eV (d) 1.282 eV

Figure S6 Top and side views of the most stable adsorption configurations with phenoxy adsorbed parallel on a terrace (a-c) and vertically (d) on the Rh(111) surface, with corresponding reaction energy (with respect to the most stable adsorption site of phenol) indicated for each structure. The black lines in the top views indicate the surface unit cells used in the calculations.



(a) Phenoxy on Pt(111)



(b) Phenoxy on Rh(111)

Figure S7 Spin-polarized PDOS of phenoxy (summed over the entire molecule) adsorbed in its most stable adsorption configurations on (a) Pt(111) and (b) Rh(111), respectively, illustrating that phenoxy is not a radical when adsorbed on the two surfaces. The blue dashed lines show the PDOS for phenol in vacuum, while the red solid lines show the PDOS for phenol adsorbed on the two surfaces. The vacuum level of the molecule in vacuum and the molecule on a surface have been aligned in the two plots. The adsorption geometries are depicted in Fig. S5a and S6a for Pt and Rh, respectively.