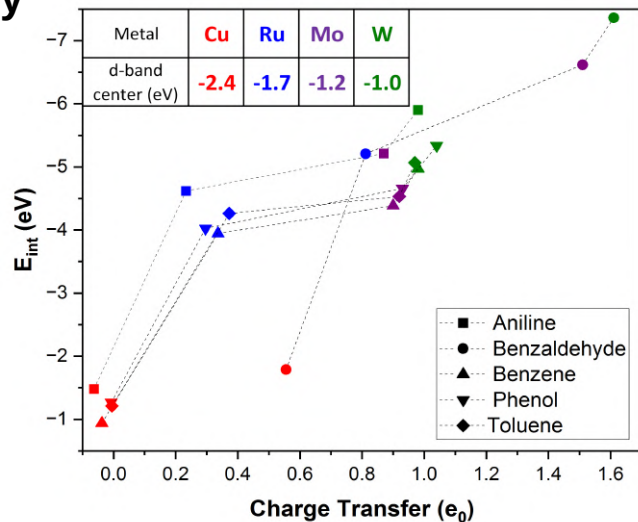
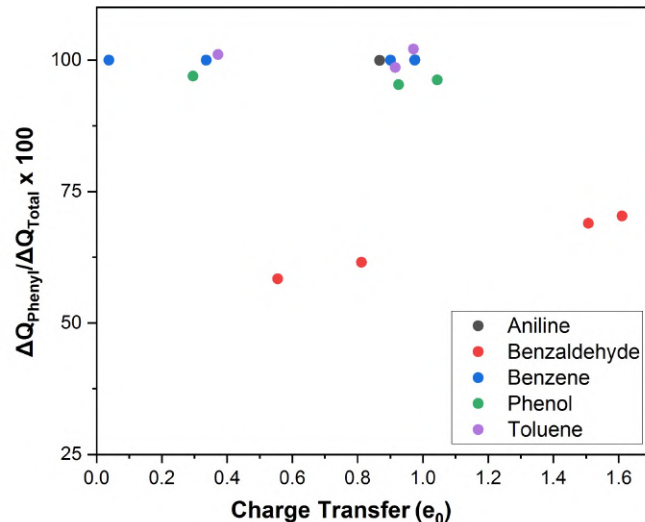


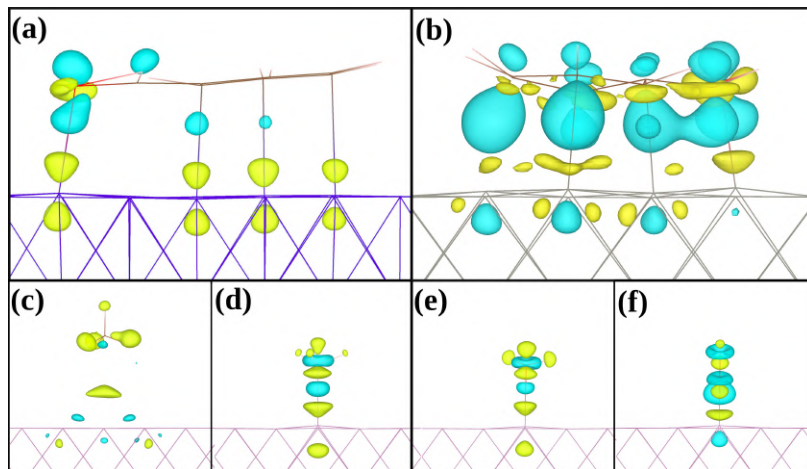
# Supplementary Information



**Fig. 1.** Relationship between transferred charge and interaction energy for all SMIs adsorbed on metal surfaces in this study. The metal surfaces are distinguished by color, while the adsorbates are represented by different symbol shapes.



**Fig. 2.** Percentage of transferred charge directed to the phenyl group of the SMIs.



**Fig. 3.** Charge difference plots.

**Top:** Benzaldehyde adsorption on **(a)** Cu and **(b)** W surfaces.  
**Bottom:** Adsorption of **(c)** CH<sub>4</sub>, **(d)** NH<sub>3</sub>, **(e)** H<sub>2</sub>O, and **(f)** CO on the Mo surface.  
 The isosurfaces (in  $e_0/\text{\AA}^3$ ) correspond to 0.01 for **(a)**, **(b)**, and **(f)**, 0.0005 for **(c)**, and 0.001 for **(d)** and **(e)**.