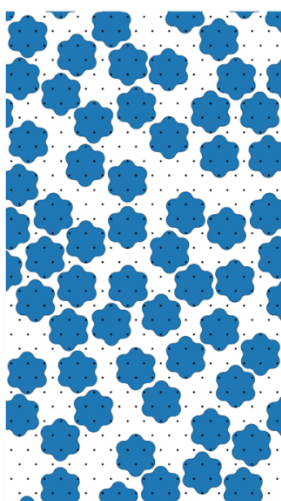


Figure 1: (left) DFT is used to determine favorable binding configurations of Hhfac on Al<sub>2</sub>O<sub>3</sub>. (mid) Top view of Hhfac with the van der Waals radii of the individual atoms. (right) Hhfac is flattened and turned into a shape to be used in RSA simulations.

(a)



(b)

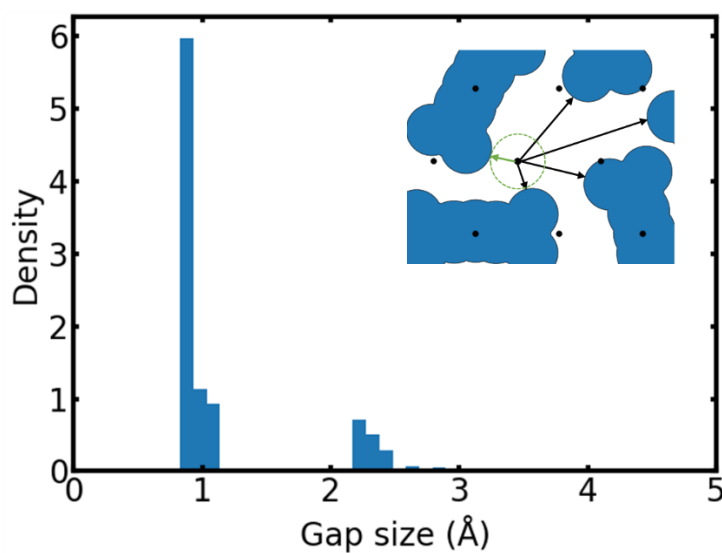


Figure 2: (a) Results of RSA simulation of benzene on Ru. (b) The capability of gaps to adsorb precursor molecules is analyzed by calculating the smallest distance from an unoccupied surface site to neighboring inhibitor molecules. The resulting gap size distribution is used to assess the precursor blocking.