An automated adsorption simulation workflow for efficient high-throughput molecule screening for area-selective deposition

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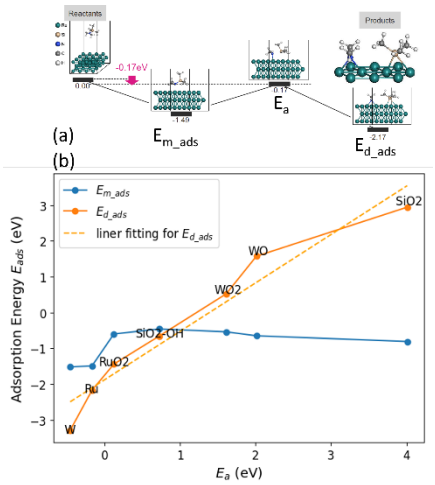

Figure 2 (a) An example of manual adsorption energy and activation energy simulation for TMSDMA on Ru substrate. (b) E_{m_ads} and E_{d_ads} for TMSDMA on different substrates compared to the corresponding activation energy E_a.

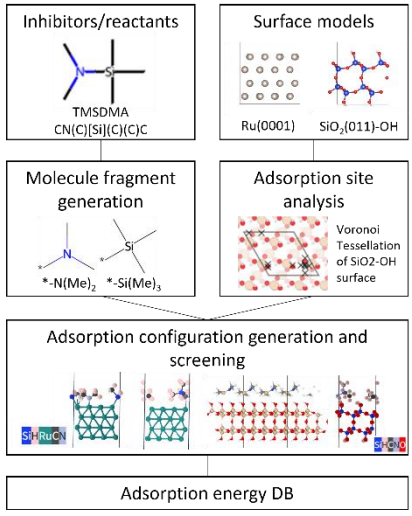

Figure 1 Schematic workflow of automatic adsorption energy simulation.

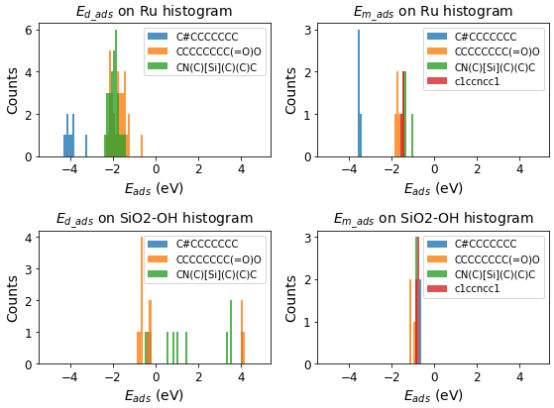

Figure 3 Histogram of adsorption energies for different adsorption configurations.

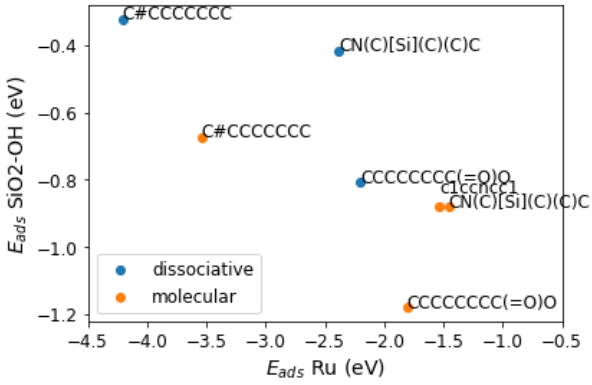

Figure 4 Adsorption energies on Ru versus SiO2-OH for the studied four type of molecules.