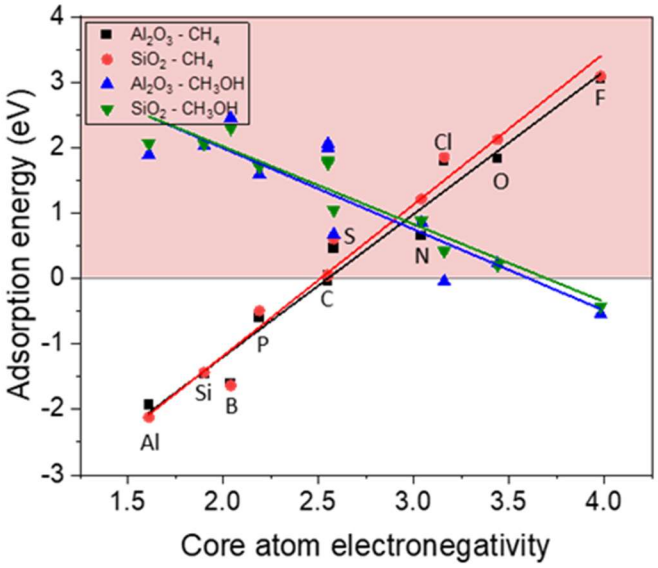

Figure 1: a) Adsorption energies versus core atom electronegativity for a variety of SMIs on oxide surfaces. Adsorption energies are calculated for chemisorption with byproduct formation of CH_4 for Al_2O_3 (black) and SiO_2 (red), and CH_3OH for Al_2O_3 (blue) and SiO_2 (green). All values above zero are highlighted in red as they are considered unfavorable.

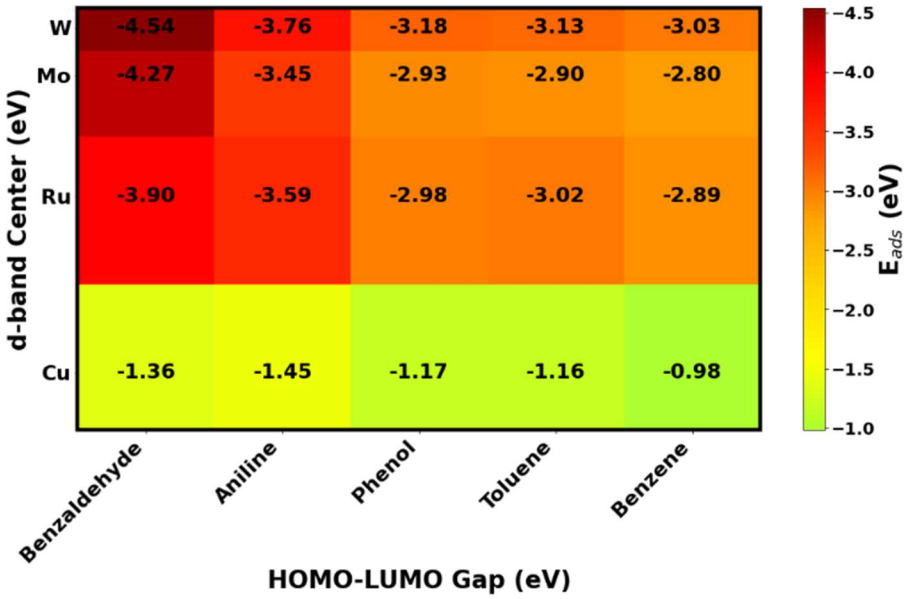

Figure 2: Adsorption energies versus d-band center and HOMO-LUMO gap for a variety of SMIs (benzaldehyde, aniline, phenol, toluene, and benzene) on metal surfaces. The color bar indicates how exothermic the adsorption energy is, from less exothermic (green) to more exothermic (red).