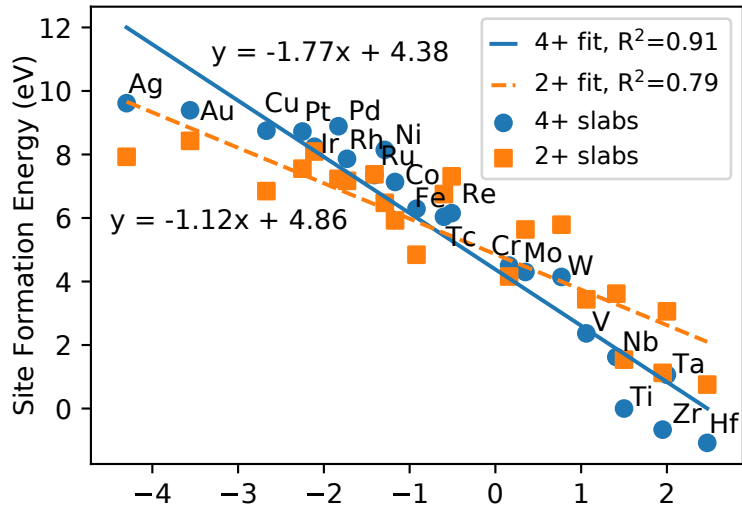


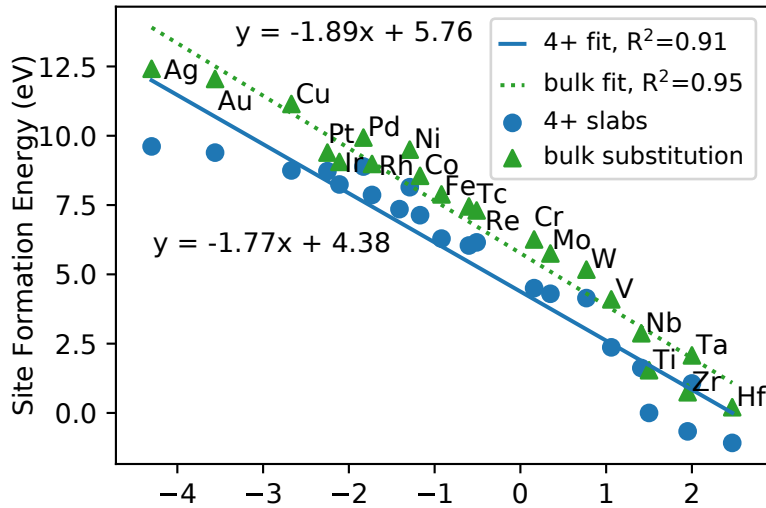
d-band Center vs Site Formation Energy



(a)

d-band Center (eV)

d-band Center vs Bulk Substitution Formation Energy



(b)

d-band Center (eV)