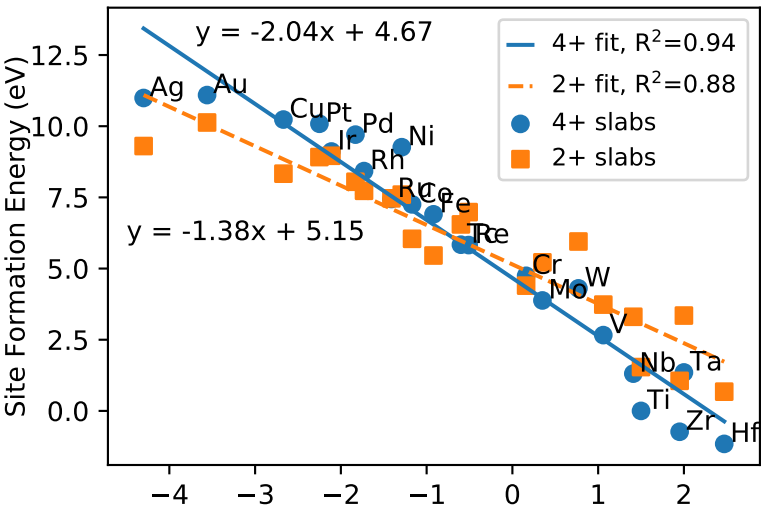
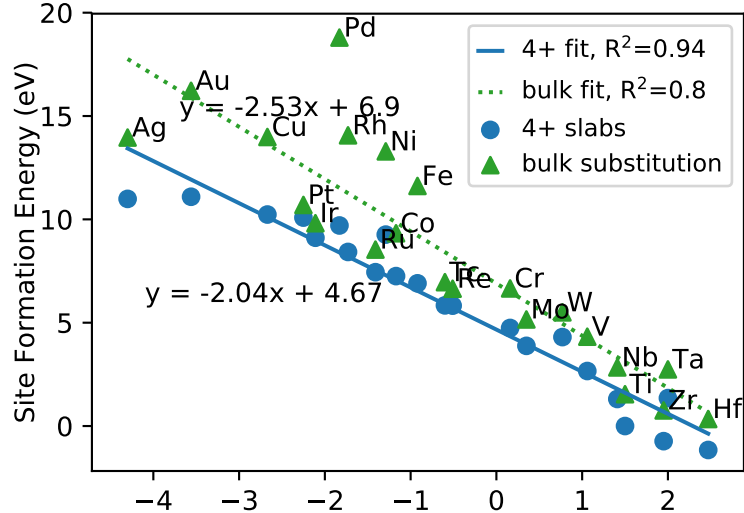


d-band Center vs Site Formation Energy

(a)
d-band Center (eV)

d-band Center vs Bulk Substitution Formation Energy

(b)
d-band Center (eV)