Modeling materials using density functional theory

By John R. Kitchin $\Delta E = 0.440 \text{ eV}$ $E^{\dagger} = 0.575 \text{ eV}$ images 0.4 Energy (eV) 0.3 0.2 0.1 Bulk Clean surface covered 20 15 2.5 10 OOS (arbitrary units) 0.0 -0.5 L $E-E_f$ (eV) -10^L k-vector -56.25 E1 parabolic fit Murnaghan fit -56.30 -56.35 Energy (eV) Min volume = $16.57 \, \text{Å}^3$ F4 E6 Bulk modulus = $0.49 \text{ eV/Å}^3 = 78.46 \text{ GPa}$ -56.40 -56 45 F3 CuPd Cu3Pd -56.50 L 18

Volume (\mathring{A}^3)