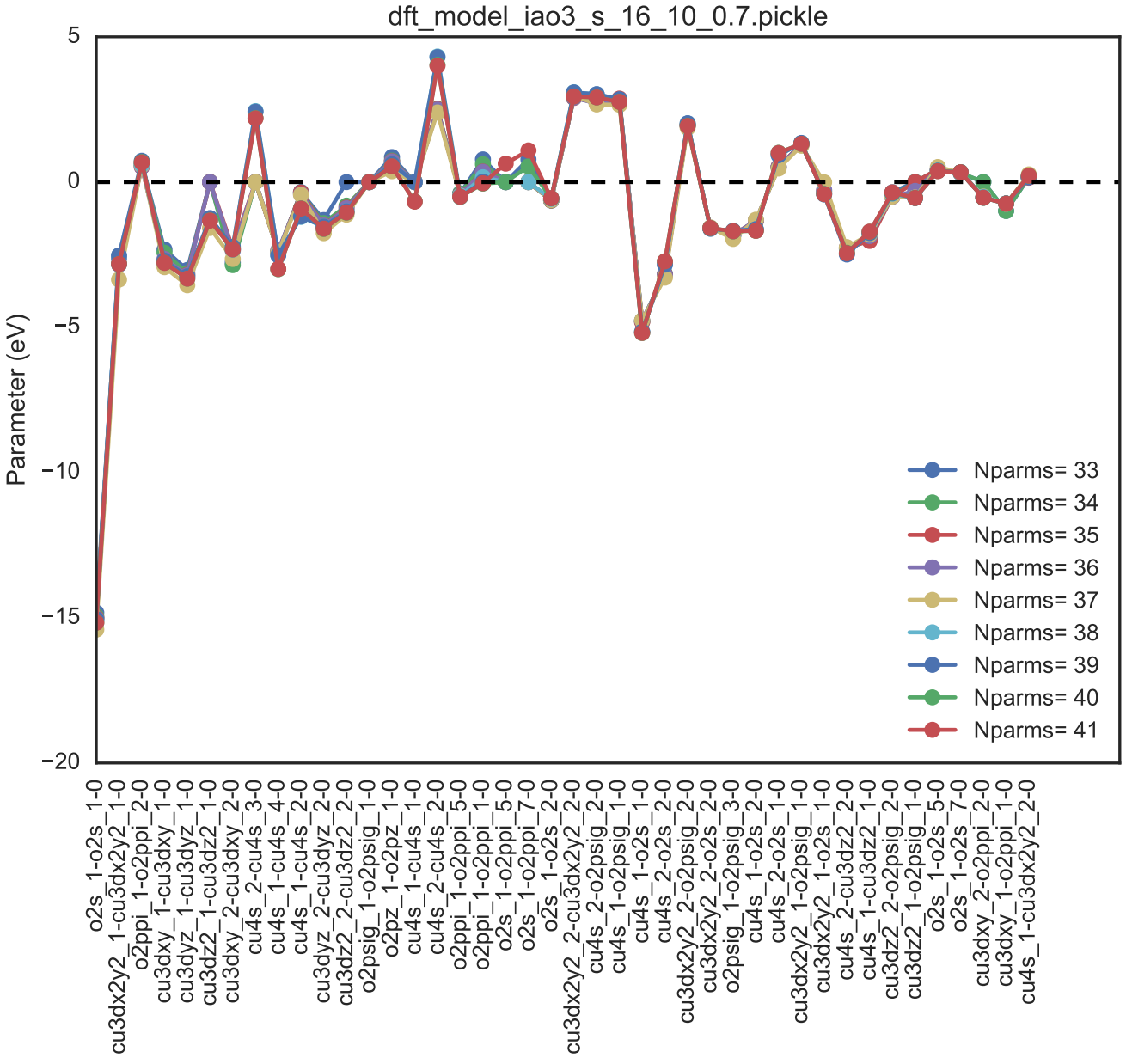
dft_model_iao3_s_16_10_0.7.pickle
Parameter (eV)
5
0
−5
−10
−15
−20
Nparms= 33
Nparms= 34
Nparms= 35
Nparms= 36
Nparms= 37
Nparms= 38
Nparms= 39
Nparms= 40
Nparms= 41
o2s_1-o2s_1-0
cu3dx2y2_1-cu3dx2y2_1-0
o2ppi_1-o2ppi_2-0
cu3dxy_1-cu3dxy_1-0
cu3dyz_1-cu3dyz_1-0
cu3dz2_1-cu3dz2_1-0
cu3dxy_2-cu3dxy_2-0
cu4s_2-cu4s_3-0
cu4s_1-cu4s_4-0
cu4s_1-cu4s_2-0
cu3dyz_2-cu3dyz_2-0
cu3dz2_2-cu3dz2_2-0
o2psig_1-o2psig_1-0
o2pz_1-o2pz_1-0
cu4s_1-cu4s_1-0
cu4s_2-cu4s_2-0
o2ppi_1-o2ppi_5-0
o2ppi_1-o2ppi_1-0
o2s_1-o2ppi_5-0
o2s_1-o2ppi_7-0
o2s_1-o2s_2-0
cu3dx2y2_2-cu3dx2y2_2-0
cu4s_2-o2psig_2-0
cu4s_1-o2psig_1-0
cu4s_1-o2s_1-0
cu4s_2-o2s_2-0
cu3dx2y2_2-o2psig_2-0
cu3dx2y2_2-o2s_2-0
o2psig_1-o2psig_3-0
cu4s_1-o2s_2-0
cu4s_2-o2s_1-0
cu3dx2y2_1-o2psig_1-0
cu3dx2y2_1-o2s_1-0
cu4s_2-cu3dz2_2-0
cu4s_1-cu3dz2_1-0
cu3dz2_2-o2psig_2-0
cu3dz2_1-o2psig_1-0
o2s_1-o2s_5-0
o2s_1-o2s_7-0
cu3dxy_2-o2ppi_2-0
cu3dxy_1-o2ppi_1-0
cu4s_1-cu3dx2y2_2-0