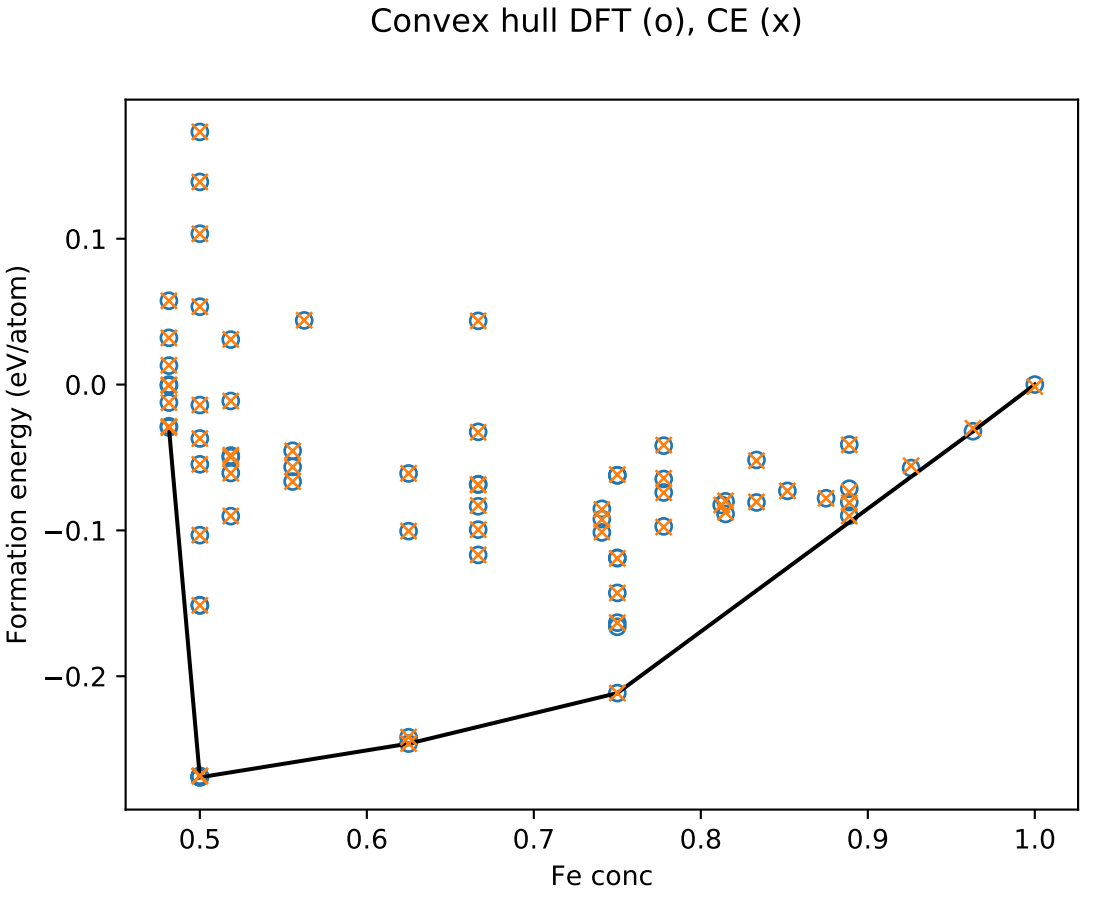
Convex hull DFT (o), CE (x)
Formation energy (eV/atom)
0.1
0.0
−0.1
−0.2
0.5
0.6
0.7
0.8
0.9
1.0
Fe conc