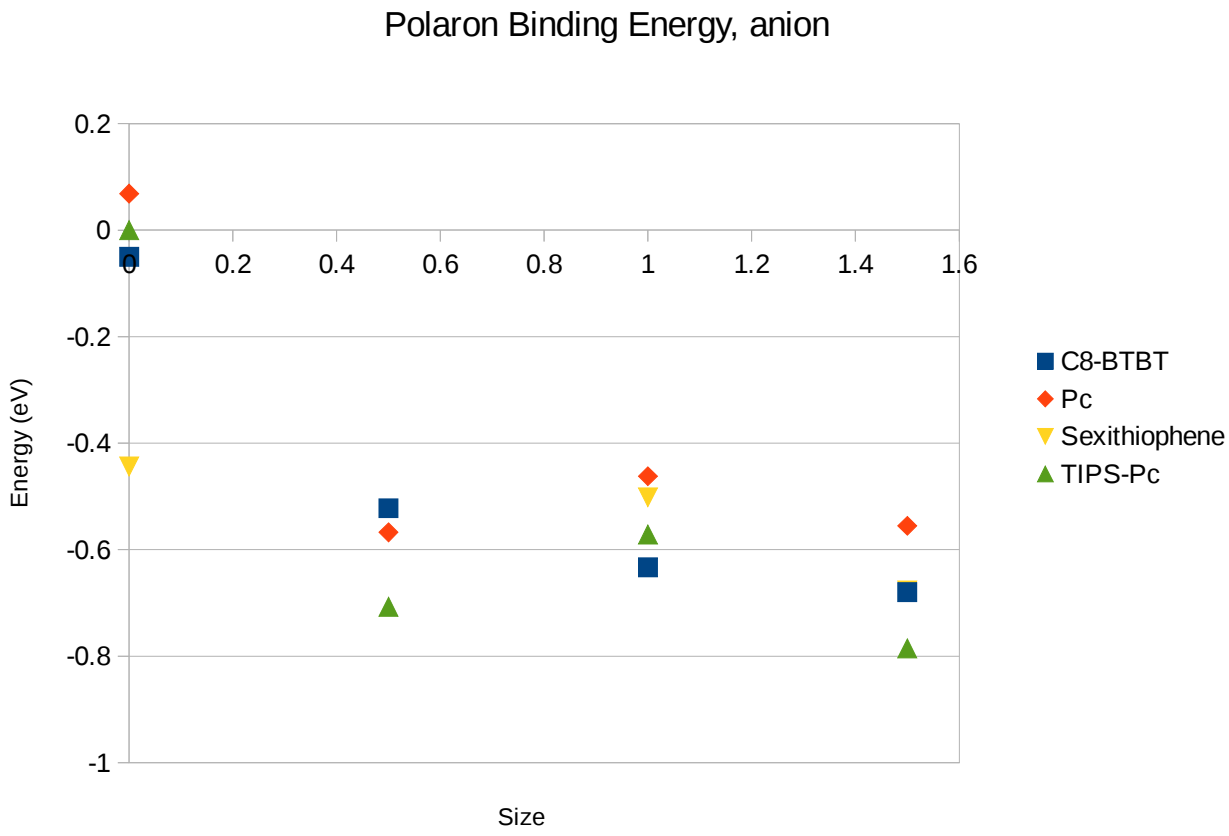
Polaron Binding Energies
4/4/14

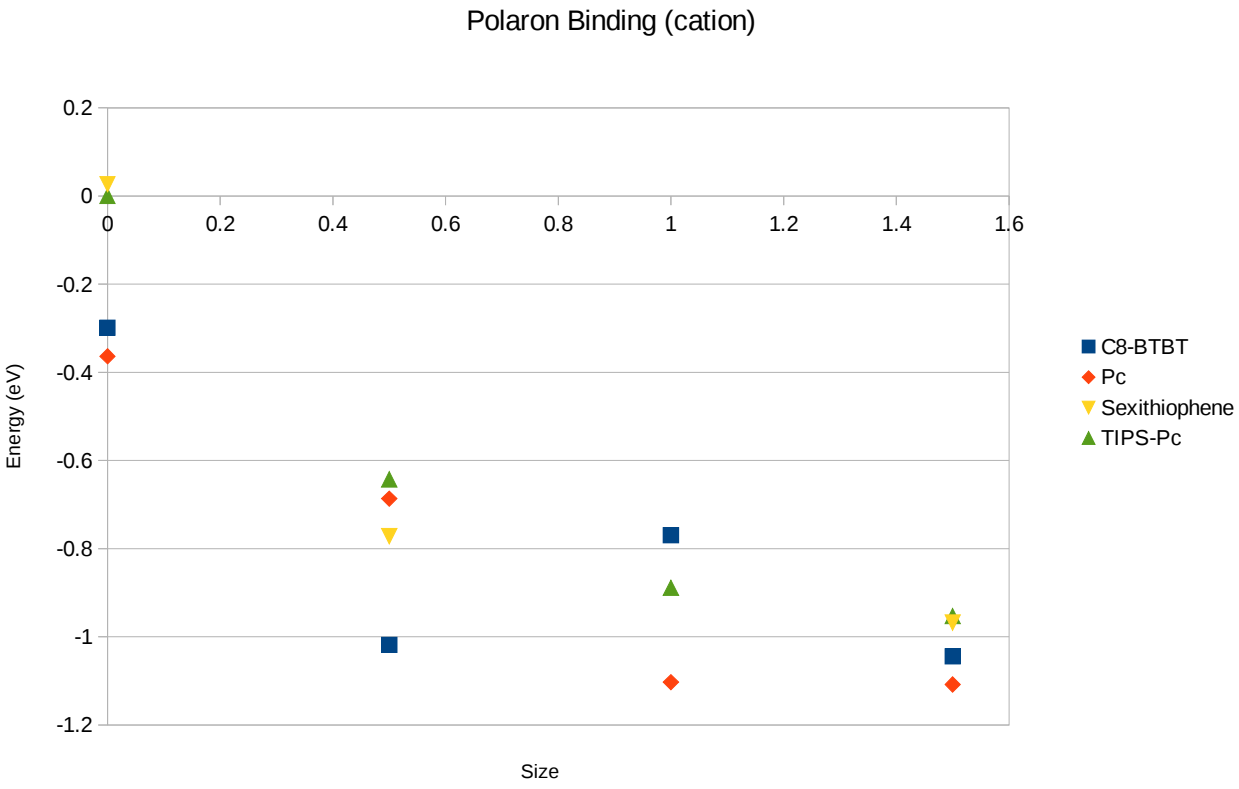
Size 0 refers to single unit cell

Size 1,2,3,4,... refer to cubes with max TVs 1,2,3,4 from central molecule in each direction

Size 0.5,1.5,2.5,3.5,4.5, refer to “diamonds” with max TOTAL TVs from centre molecule of 1,2,3,4...

Values are reasonably consistent with size(+/- ~0.15eV), and some resonance with cube/diamond in some cases. Cation bindings seem to be slightly stronger and take longer to converge... Not sure why, distribution of charge is different from anion though. Perhaps more charge density close to extremities of moluecule, giving more polar response?




Polaron Binding (cation)
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-1.2
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
Energy (eV)
Size
C8-BTBT
Pc
Sexithiophene
TIPS-Pc