

ECP and basis sets for O and Cu used in this study (in CRYSTAL format).

```

O basis set
8 6
0 0 6 2.0 1.0
8588.5000000      0.00189515
1297.2300000      0.0143859
299.2960000       0.0707320
87.3771000        0.2400010
25.6789000        0.5947970
3.7400400         0.2808020
0 1 3 6.0 1.0
42.1175000        0.1138890      0.0365114
9.6283700         0.9208110      0.2371530
2.8533200         -0.00327447    0.8197020
0 1 1 0.0 1.0
0.9359510         1.0000000      1.0000000
0 1 1 0.0 1.0
0.3343400         1.0000000      1.0000000
0 1 1 0.0 1.0
0.1209990         1.0000000      1.0000000
0 3 1 0.0 1.0
1.0366040         1.0000000
Cu ECP and basis set
229 7
INPUT
19.0 1 3 2 0 0 0
23.2906000        -4.0027600      -1
2.6205900         3.3246500      -2
7.8108200         224.3233000     0
6.6332400         -180.3047000    0
51.1573400        3.4213000      -2
14.7340600        105.7012600     0
0 1 4 8.0 1.0
83.4200000        -0.0041850     -0.0068680
7.9700000         -0.4107060     -0.2744770
5.6000000         0.0307600      0.5327810
1.9320000         0.6904310      0.6238650
0 1 1 1.0 1.0
2.9849300         1.0000000      1.0000000
0 1 1 0.0 1.0
0.7025260         1.0000000      1.0000000
0 1 1 0.0 1.0
0.1705310         1.0000000      1.0000000
0 3 4 10.0 1.0
65.8000000        0.0169140
18.8200000        0.1069740
6.5380000         0.2875190
2.3480000         0.4097730
0 3 1 0.0 1.0
0.8012300         1.0000000
0 3 1 0.0 1.0
0.2398190         1.0000000

```