Supporting information for: "Thermoelectric Properties of p-type Cu_2O, CuO, and NiO from Hybrid Density Functional Theory"

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Contents

1 Basis set information

In periodic calculations, the Gaussian-type localized atomic basis set must be chosen carefully. Basis sets originally developed for molecular calculations contain diffuse basis functions to model the tails of the wavefunction, but in periodic calculations, where the whole space is filled with basis functions, such diffuse functions are usually unnecessary and lead into numerical difficulties and/or severe degradation of performance.[1] The basis sets used in this work were obtained as follows:

Cu,O: Basis sets for Cu and O are described in previous studies.[2,3]
Ni: The TZVP basis set for Ni was derived from the molecular Karlsruhe def-TZVP basis set.[4] The diffuse outermost s-exponents were increased from 0.0468 and 0.133 to 0.14 and 0.35, respectively. The exponent of the p-type polarization function was changed from 0.147 to 0.14 and the outermost s and p functions were then combined into a single sp-type function.

TZVP basis set for nickel listed as CRYSTAL17 input format:

```
28 12
0 0 8 2.0 1.0
351535.72935      .22529386884E-03
52695.809283      .17468616223E-02
11992.468293      .90849992136E-02
3394.5776689      .36940748447E-01
1105.3594585      .12032819950
397.14677769      .28596715057
154.27542974      .40983020196
61.018723780      .21620642851
0 0 4 2.0 1.0
384.45559739     -.24651279268E-01
119.04879199     -.11658505277
19.137012223      .54864126676
8.1526718562      .52640051122
0 0 2 2.0 1.0
12.579408642     -.22797884293
2.0870866081      .70703738215
0 0 1 1.0 1.0
0.86432568555     1.0000000000
0 0 1 0.0 1.0
0.35              1.0000000000
0 1 1 0.0 1.0
0.14              1.0 1.0
0 2 6 6.0 1.0
1883.0907486      .23748258443E-02
445.95155320      .19289457172E-01
143.08430815      .90718211507E-01
53.372920722      .26181414117
21.321919357      .42309149832
8.6643561994      .24641686015
0 2 3 6.0 1.0
34.144255211     -.29677129163E-01
4.7122455921      .55616824096
1.8709231845      .96357766460
0 2 1 0.0 1.0
0.70370016267      1.0000000000
0 3 4 9.0 1.0
```

```
74.591603465       .12077454672E-01
21.590632752       .74637262154E-01
7.6246142580       .23236775502
2.8632206762       .39042651680
0 3 1 0.0 1.0
1.0311063388       .39509498921
0 3 1 0.0 1.0
0.33060760691      .21138769167
```

2 Comparison of CRYSTAL17 and BoltzTraP for calculating transport properties of CuO and NiO

As mentioned in the paper, results between the two methods for calculating the transport properties are almost indistinguishable, as seen in Figures 1 and 2.

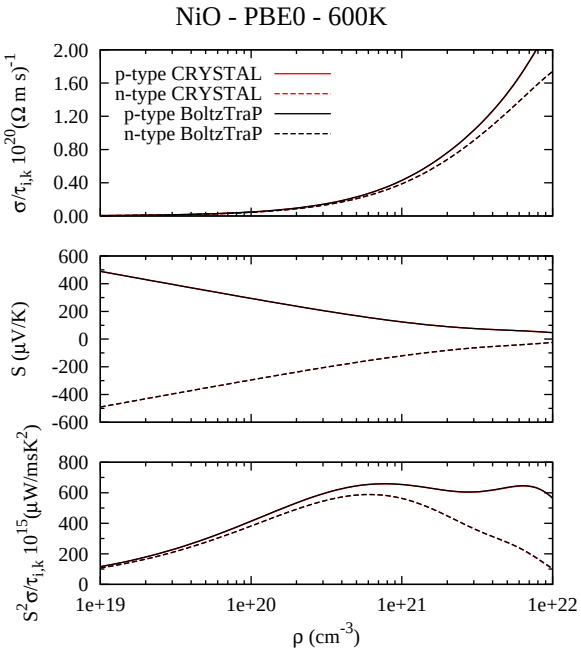

Figure 1: Transport coefficients for NiO as a function of carrier concentration ρ calculated with CRYSTAL17 and BoltzTraP. Top: Electrical conductivity calculated with the electronic relaxation time as a free parameter. Middle: Seebeck coefficient. Bottom: Power factor $S^2\sigma$.

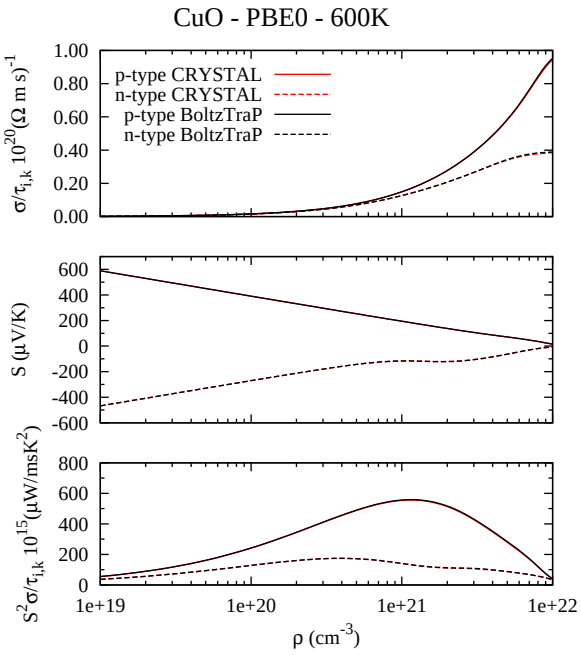

Figure 2: Transport coefficients for CuO as a function of carrier concentration ρ calculated with CRYSTAL17 and BoltzTraP. Top: Electrical conductivity calculated with the electronic relaxation time as a free parameter. Middle: Seebeck coefficient. Bottom: Power factor $S^2\sigma$.

3 Optimized geometries of Cu_2O, CuO and NiO

Optimized cell parameters and atomic positions are given below in CRYSTAL input format. CuO and NiO are given in the supercell geometry. The spin configuration for the metal atoms in CRYSTAL ATOMSPIN format is 1, -1, 1, -1 for CuO and 1, -1 for NiO.

Cu_2O:

```
CRYSTAL
0 0 0
224
4.31752282
2
29 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
8  2.500000000000E-01 2.500000000000E-01 2.500000000000E-01
```

CuO:

```
CRYSTAL
0 0 0
7
7.55422533 3.42947873 6.38035080 94.856999
8
29 -1.205306609048E-01 1.467042653708E-03 -1.229445962040E-01
29 3.794697971259E-01 1.471030022252E-03 3.770566294213E-01
29 1.280914668936E-01 4.986670078364E-01 1.267625033871E-01
29 -3.719177816402E-01 4.987626020411E-01 -3.732588786610E-01
8 1.292168618829E-01 1.650934187911E-01 -1.233320535690E-01
```

```
8 -3.707864909944E-01 1.650937001219E-01 3.766938213238E-01
8 3.784286868259E-01 -3.349205574054E-01 1.273116508464E-01
8 -1.215718791889E-01 -3.349020590435E-01 -3.726890765446E-01
```

NiO:

```
CRYSTAL
0 0 0
166
2.96323108 14.48172881
3
28 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
28 0.000000000000E+00 0.000000000000E+00 5.000000000000E-01
8  3.333333333333E-01 -3.333333333333E-01 -8.333344676109E-02
```

References

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