# Supporting Information

# DFTB parameters for the Periodic Table: part III, Spin-Orbit Coupling

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## Spin-Orbit Coupling Parameters

**Table 1**. Renormalized Spin-orbit coupling parameters calculated at GGA-PBE/SOC-ZORA/AE theory level. All values are in milli-Hartrees.

| | ε(p) | ε(d) | ε(f) | | ε(p) | ε(d) | ε(f) | | ε(p) | ε(d) | ε(f) | | ε(p) | ε(d) | ε(f) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **H** | __ | __ | __ | **Ga** | 3.93 | __ | __ | **Pm** | 112.6 | 3.83 | 5.38 | **Pa** | 207.12 | 7.24 | 61.41 |
| **He** | __ | __ | __ | **Ge** | 6.32 | __ | __ | **Sm** | 121.0 | 3.98 | 6.11 | **U** | 244.96 | 7.68 | 73.13 |
| **Li** | __ | __ | __ | **As** | 9.21 | __ | __ | **Eu** | 129.7 | 4.13 | 6.89 | **Np** | __ | __ | __ |
| **Be** | __ | __ | __ | **Se** | 12.63 | __ | __ | **Gd** | 138.8 | 4.27 | 7.71 | **Pu** | __ | __ | __ |
| **B** | 0.12 | __ | __ | **Br** | 16.65 | __ | __ | **Tb** | 148.4 | 4.40 | 8.59 | **Am** | __ | __ | __ |
| **C** | 0.31 | __ | __ | **Kr** | 21.30 | __ | __ | **Dy** | 158.3 | 4.52 | 9.53 | **Cm** | __ | __ | __ |
| **N** | 0.68 | __ | __ | **Rb** | 29.33 | __ | __ | **Ho** | 168.7 | 4.63 | 10.53 | **Bk** | __ | __ | __ |
| **O** | 1.29 | __ | __ | **Sr** | 38.61 | __ | __ | **Er** | 179.6 | 4.73 | 11.58 | **Cf** | __ | __ | __ |
| **F** | 2.24 | __ | __ | **Y** | 48.24 | 1.44 | __ | **Tm** | 191.0 | 4.82 | 12.71 | **Es** | __ | __ | __ |
| **Ne** | 3.62 | __ | __ | **Zr** | 58.69 | 2.13 | __ | **Yb** | 203.0 | 4.90 | 13.89 | **Fm** | __ | __ | __ |
| **Na** | 6.23 | __ | __ | **Nb** | 69.15 | 2.55 | __ | **Lu** | 215.5 | 4.97 | __ | **Md** | __ | __ | __ |
| **Mg** | 9.99 | __ | __ | **Mo** | 81.64 | 3.35 | __ | **Hf** | 242.8 | 7.01 | __ | **No** | __ | __ | __ |
| **Al** | 0.57 | __ | __ | **Tc** | 96.65 | 4.69 | __ | **Ta** | 272.7 | 9.11 | __ | **Lr** | 551.55 | 9.33 | __ |
| **Si** | 1.11 | __ | __ | **Ru** | 110.5 | 5.26 | __ | **W** | 305.2 | 11.33 | __ | **Rf** | 612.09 | 13.07 | __ |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **P** | 1.87 | __ | __ | **Rh** | 127.0 | 6.39 | __ | **Re** | 340.4 | 13.69 | __ | **Db** | 677.68 | 16.73 | __ |
| **S** | 2.92 | __ | __ | **Pd** | 143.8 | 7.07 | __ | **Os** | 378.2 | 16.20 | __ | **Sg** | 748.40 | 20.47 | __ |
| **Cl** | 4.30 | __ | __ | **Ag** | 164.7 | 9.02 | __ | **Ir** | 418.8 | 18.89 | __ | **Bh** | 824.43 | 24.35 | __ |
| **Ar** | 6.08 | __ | __ | **Cd** | 188.1 | 11.25 | __ | **Pt** | 458.7 | 20.43 | __ | **Hs** | 905.99 | 28.38 | __ |
| **K** | 9.20 | __ | __ | **In** | 10.32 | __ | __ | **Au** | 505.0 | 23.40 | __ | **Mt** | 993.39 | 33.81 | __ |
| **Ca** | 13.19 | __ | __ | **Sn** | 14.69 | __ | __ | **Hg** | 558.4 | 28.07 | __ | **Ds** | 1087.0 | 37.02 | __ |
| **Sc** | 17.46 | 0.52 | __ | **Sb** | 20.05 | __ | __ | **Tl** | 32.76 | __ | __ | **Rg** | 1187.1 | 41.64 | __ |
| **Ti** | 22.45 | 0.79 | __ | **Te** | 26.08 | __ | __ | **Pb** | 46.13 | __ | __ | **Cn** | 1294.1 | 48.62 | __ |
| **V** | 28.28 | 1.12 | __ | **I** | 32.82 | __ | __ | **Bi** | 60.46 | __ | __ | **Nh** | 93.31 | __ | __ |
| **Cr** | 34.44 | 1.31 | __ | **Xe** | 40.33 | __ | __ | **Po** | 75.98 | __ | __ | **Fl** | 125.51 | __ | __ |
| **Mn** | 42.88 | 1.99 | __ | **Cs** | 53.23 | __ | __ | **At** | 92.82 | __ | __ | **Mc** | 159.60 | __ | __ |
| **Fe** | 51.86 | 2.56 | __ | **Ba** | 67.51 | __ | __ | **Rn** | 111.1 | __ | __ | **Lv** | 196.28 | __ | __ |
| **Co** | 62.09 | 3.22 | __ | **La** | 81.52 | 3.06 | 2.88 | **Fr** | 141.9 | __ | __ | **Ts** | 235.98 | __ | __ |
| **Ni** | 72.77 | 3.64 | __ | **Ce** | 89.01 | 1.96 | 3.46 | **Ra** | 175.0 | __ | __ | **Og** | 278.99 | __ | __ |
| **Cu** | 85.78 | 4.49 | __ | **Pr** | 96.63 | 3.47 | 4.06 | **Ac** | 141.3 | 5.86 | __ | | | | |
| **Zn** | 101.5 | 5.90 | __ | **Nd** | 104.5 | 3.66 | 4.70 | **Th** | 174.2 | 8.14 | 50.37 | | | | |

**Spin-Orbit Coupling Parameters (D.J. Chadi)[1]**

**Table 2**. Renormalized Spin-orbit coupling parameters of valence p state calculated using a Tight Binding approach. All values are in milli-Hartrees.

| | **ε(p)** | | **ε(p)** |
|---|---|---|---|

| | | | |
|---|---|---|---|
| **Al** | 0.88 | **As** | 15.47 |
| **Si** | 1.61 | **Se** | 17.63 |
| **P** | 2.46 | **Cd** | 8.34 |
| **S** | 2.71 | **In** | 14.40 |
| **Zn** | 2.71 | **Sn** | 29.40 |
| **Ga** | 6.39 | **Sb** | 35.75 |
| **Ge** | 10.65 | **Te** | 40.42 |

## Crystal Structure Information

**Table 3.** Geometric parameters of the reference structures along with the lattice information. Lattice parameters are a, b, and c; d is the interplanar distance. All values are in Å

| | **Lattice** | **a** | **b** | **c** | **d** |
|---|---|---|---|---|---|
| **GaAs** | Cubic | 3.981 | 3.981 | 3.981 | __ |
| **InSb** | Cubic | 4.582 | 4.582 | 4.582 | __ |
| **ZnSe** | Cubic | 4.009 | 4.009 | 4.009 | __ |
| **Si** | Cubic | 3.840 | 3.840 | 3.840 | __ |
| **Ge** | Cubic | 4.002 | 4.002 | 4.002 | __ |
| **$MoS_2$** | Hexagonal | 3.16 | 3.16 | __ | __ |
| **$MoSe_2$** | Hexagonal | 3.19 | 3.29 | __ | __ |
| **$WS_2$** | Hexagonal | 3.15 | 3.15 | __ | __ |
| **$WSe_2$** | Hexagonal | 3.18 | 3.28 | __ | __ |
| **Me-Bi** | Hexagonal | 5.497 | 5.497 | __ | 0.054 |
| **Me-Sb** | Hexagonal | 5.253 | 5.253 | __ | 0.032 |
| **Me-Pb** | Hexagonal | 5.026 | 5.026 | __ | 0.855 |

**Structural Parameters DOI:** https://doi.org/10.5281/zenodo.6461821

## References

(1) Chadi, D. J. Spin-orbit splitting in crystalline and compositionally disordered semiconductors. *Physical Review B* **1977**, *16* (2), 790. DOI: 10.1103/PhysRevB.16.790.