Supplementary material to ”Assessing the Performance of Recent Density Functionals for Bulk Solids”

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(Dated: February 20, 2009)

Parameters of the PAW data sets used in the present work. In all cases, two partial waves are used for the *s* and *p* orbitals. “valence” indicates which orbitals are treated as valence electrons; rcl are the cutoff radii for the partial waves. If small indices are used, they indicate which cutoff was used for *s*-, *p*-, and *d*-partial waves. Ecut are the energy cutoffs for which Ekin < 0.1 mRy. For further details, the authors refer to Refs. 42 and 48 of the present work.

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|  | **Valence** | **rcl (a.u.)** | **Ecut (eV)** |
| **Li** | 1s2s2p | 1.7 | 500 |
| **C** | 2s2p | 1.2s, 1.5p | 400 |
| **O**  | 2s2p | 1.2s, 1.52p | 400 |
| **F** | 2s2p | 1.2s, 1.52p | 400 |
| **Na** | 2p3s | 2.2 | 260 |
| **Mg**  | 3s3p | 2.0 | 270 |
| **Al** | 3s3p | 1.9 | 245 |
| **Si** | 3s3p | 1.9 | 250 |
| **Cl** | 3s3p | 1.9 | 280 |
| **K**  | 3s3p4s | 2.3 | 260 |
| **Ca**  |  3p4s  | 3 | 150 |
| **Cu** | 3d4s | 2.3 | 295 |
| **Ga**  | 3d4s4p | 2.3 | 285 |
| **Ge** | 3d4s4p | 1.6d, 2.3s,p | 580 |
| **As** | 4s4p | 2.1 | 210 |
| **Rb**  |  4p5s  | 3.3 | 122 |
| **Sr**  |  4s4p5s  | 2.5 | 226 |
| **Rh** | 4p4d5s5p | 2.1p, 2.4s,d | 250 |
| **Pd** | 4p4d5s5p | 2.1p, 2.4s,d | 255 |
| **Ag** | 4d5s | 2.4s,d | 250 |
| **Cs**  |  5s5p6s  | 1.9s, 2.5p,d  | 221 |
| **Ba**  |  5s5p6s  |  2.8s, 2.7p,d  | 187 |
| **Pb**  |  5d6s6p  | 2.5 | 238 |