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Introduction



The [Presentations](#) investigate the accuracy of a range of different [DFT: LCAO](#) electronic-structure methods in calculations for bulk semiconductors. In particular, we apply GGA and MGGA exchange-correlation functionals, as well as the [Pseudopotential Projector-Shift](#) method. Some comparisons to [HSE](#) results are also included.

Both structural and electronic quantities are computed and the different methods are benchmarked against each other. Computational settings such as k -point sampling and density mesh cutoff energy are also considered.

Note

The [Presentations](#) are continuously expanded with more data and more semiconductors.

All calculations are done using the newest updates (August 2016) to the [SG15/PseudoDojo](#) pseudopotentials and basis sets. The applied exchange-correlation functionals usually include PBE, PBEsol, TB09-MGGA, and PBE augmented with the PPS method. Each combination of pseudopotential, basis set, and exchange-correlation functional constitutes a **computational method**.

The following **structural and electronic quantities** are considered:

- Lattice constant(s)
- Elastic constants
- Band structure
- Band gaps
- Effective masses
- Dielectric constant(s)

Extensive **convergence studies** are conducted for the different computational methods. In particular, the convergence of the lattice constant, bulk total energy and band gap is thoroughly studied with respect to k -point sampling and density mesh cutoff energy.

Methods

The [SG15/PseudoDojo](#) normconserving pseudopotentials were recently implemented in the [DFT: LCAO](#) calculator engine. This suite of pseudopotentials was generated using the Optimized Norm-Conserving

Vanderbilt (ONCV) method, as described in [1] and [2]. More information is available on the [SG15-ONCV website](#).

As explained in the document [Pseudopotentials and basis sets available in QuantumATK](#), three different QuantumATK basis sets are available for each element when using the SG15 pseudopotentials, with increasing accuracy; **Medium**, **High**, and **Ultra**. All three derive from the numerical atom-centered basis sets of the [FHI-aims](#) package, but have been significantly modified and optimized with respect to computational speed with the ATK-DFT calculator.

The Medium basis set is default for the SG15 pseudopotentials, and should be sufficient for most applications. However, if extreme accuracy is needed, the High and Ultra basis sets add more basis functions at the expense of increased computational load. The Ultra basis set is exceptionally large, and will usually add only little extra accuracy as compared to the High basis set, but at a fairly high extra computational cost. The Medium and High basis sets will in most cases constitute a better trade-off between computational accuracy and speed, so these are the two SG15 basis sets used in the [Presentations](#).

HSE

The HSE06 screened hybrid density functional [3] is implemented in the FHI-aims package. The “Tier 1” basis set is used with both “Light” and “Tight” accuracy settings, here denoted “l1” and “t1”, respectively.

Nomenclature

Each computational method is specified by a combination of exchange-correlation functional, pseudopotential, and basis set. Since this study uses only the SG15 pseudopotentials, this is omitted from the naming of a method. For example, a PBE calculation with the Medium basis set is simply denoted “PBE-m”. If a calculation with some method was not done at the lattice constant computed with that method, it is indicated in a paranthesis, e.g. “PBEsol(PBE)-h” for PBEsol-h at the PBE-h lattice constant.

Note

The ATK-DFT density mesh cutoff and k -point sampling used in a calculation are not contained in the naming scheme described above. One single choice of mesh cutoff and k -point sampling is determined in a convergence study.

Pseudopotential Projector-Shift

The Pseudopotential Projector-Shift (PPS) method for ATK-DFT was introduced with QuantumATK 2017. The method introduces shifts to the angular momentum projector channels used for constructing the pseudopotential, which affects the theoretical predictions obtained with standard exchange-correlation functionals, e.g. band gaps and equilibrium lattice constants. The projector shifts are essentially free parameters, which can be fitted against relevant data and used in ATK-DFT calculations, e.g. to obtain better band gaps with otherwise ordinary PBE.

The projector-shifted pseudopotential, $V_{\text{ps}}(\mathbf{r})$, is written

$$V_{\text{ps}}(\mathbf{r}) = V_{\text{ps}}^{\text{loc}}(\mathbf{r}) + \sum_{\alpha\beta} |\alpha\rangle [V_{\alpha\beta} + U_{\alpha\beta}] \langle\beta|,$$

where

$V_{\text{ps}}^{\text{loc}}$ is the local part of the pseudopotential,

$V_{\alpha\beta}$ the pseudopotential coupling matrix, and

$U_{\alpha\beta}$ the pseudopotential projector-shift matrix. The sum runs over projectors α and β .

All entries in the matrix

$U_{\alpha\beta}$ are zero when performing a standard GGA calculation, while the PPS method adds projector shifts along the matrix diagonal. These entries correspond to different angular momentum channels; s , p , d , f , etc. Only the s and p channels are relevant for silicon, which has no d -electrons, while both s , p and d are relevant for other elements, e.g. germanium. Choosing the projector shifts to use for a particular exchange-correlation functional is then a matter of fitting the shifts, or manually tuning them.

References

[1]

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[3]

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