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Doping methods available in QuantumATK

Doping methods available in QuantumATK

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The effect of electrostatic doping is generally modelled by either increasing (n-doping) or decreasing (p-doping) the number of electrons of the system with respect to the neutral case. QuantumATK offers two general methods to introduce electrostatic doping. Both lead to the same additional electrons (holes) introduced in the system, but differ in the way these extra electrons (holes) are redistributed within it.

General background

In QuantumATK the [ElectronDensity](#) of the system is expressed as a sum of two contributions:

$$\rho(\mathbf{r}) = \Delta\rho(\mathbf{r}) + \sum_i^{N_{atoms}} \rho_i^{atom}(\mathbf{r}).$$

$\Delta\rho(\mathbf{r})$ is the [ElectronDifferenceDensity](#), which for a neutral system integrates to zero:

$$\int \Delta\rho(\mathbf{r}) d\mathbf{r} = 0.$$

$\sum_i^{N_{atoms}} \rho_i^{atom}(\mathbf{r})$ is the sum of the densities associated with the individual atoms. For a neutral system, this sum integrates to the total number of electrons N :

$$\sum_i^{N_{atoms}} \int \rho_i^{atom}(\mathbf{r}) d\mathbf{r} = N.$$

It follows that the number of electrons in a generic system with charge Q , which is the integral over the electron density in real space, can be also expressed as:

$$\int \rho(\mathbf{r}) d\mathbf{r} = \tilde{N} + \sum_i^{N_{atoms}} \int \rho_i^{atom}(\mathbf{r}) d\mathbf{r}$$

where

\tilde{N} are the extra electrons leading to a charge $Q = -e \cdot \tilde{N}$. It follows that

$$\int \Delta\rho(\mathbf{r}) d\mathbf{r} = \tilde{N}.$$

In QuantumATK, the system can be doped in two different ways, either by adding an [Explicit charge](#) or by adding [Atomic compensation charges](#). The former modifies the value of \tilde{N} , whereas the latter modifies the value of N . However, both lead to the following result:

$$-e \int \Delta\rho(\mathbf{r}) d\mathbf{r} = Q.$$

Explicit charge

An explicit charge can be added by setting the `charge` parameter to a value Q in the [LCAOCalculator](#). In this case,

\tilde{N} is set to a non-zero value

$\tilde{M} = -Q/e$. The total number of electrons in the system is then determined by

$$\int \rho(\mathbf{r}) d\mathbf{r} = \tilde{N} + \sum_i^{N_{atoms}} \int \rho_i^{atom}(\mathbf{r}) d\mathbf{r} = \tilde{M} + N.$$

Note

There are two important consequences of using this method:

- The densities of the individual atoms $\rho_i^{atom}(\mathbf{r})$ are those associated with the individual neutral species;
- The extra charge is not bound to any atom. Therefore, it will redistribute in order to minimize the total energy of the system.

Atomic compensation charges

Using the [AtomicCompensationCharge](#) method,

\tilde{N} is set to zero, but the density of the i -th atom is rescaled by a factor:

$$c_i = \frac{\tilde{n}_i + n_i}{n_i}.$$

where

n_i and

\tilde{n}_i are the number of valence electrons and the extra compensation charge associated with the i -th isolated atom. The individual values of

\tilde{n}_i , and therefore the individual coefficients

c_i , can be set arbitrarily from atom to atom, even within the same chemical species. For sake of comparison, we assume here that they are all the same and that they sum up to

\tilde{M} :

$$\sum_i^{N_{atoms}} \tilde{n}_i = \tilde{M}.$$

In this case, the integral of the total density can be expressed as a sum over the individual densities

$$\int \rho(\mathbf{r}) d\mathbf{r} = \sum_i^{N_{atoms}} \int \tilde{\rho}_i^{atom}(\mathbf{r}) d\mathbf{r}$$

where

$$\tilde{\rho}_i^{atom}(\mathbf{r}) = c_i \cdot \rho_i^{atom}(\mathbf{r})$$

Due to the use of the rescaled atomic densities

$\tilde{\rho}_i^{atom}(\mathbf{r})$, the electronic density of the system will be the same as that obtained using an explicit doping:

$$\sum_i^{N_{atoms}} \int \tilde{\rho}_i^{atom}(\mathbf{r}) d\mathbf{r} = \sum_i^{N_{atoms}} \int \frac{\tilde{n}_i}{n_i} \rho_i^{atom}(\mathbf{r}) d\mathbf{r} + \sum_i^{N_{atoms}} \int \rho_i^{atom}(\mathbf{r}) d\mathbf{r} = \tilde{N} + N$$

Note

Using this method, the extra charge is introduced by modifying the densities of the individual atoms. As a consequence:

- The extra electron density will be bound to those atoms for which $n_i \neq 0$;
- The electrostatic potential will be locally modified in the vicinity of such charged atoms, becoming more attractive (repulsive) if $n_i > 0$ ($n_i < 0$).

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