Format of the v1.0 Slater-Koster files

1 Introduction

Every Slater-Koster file distributed from the DFTB.ORG site (with the file extension '.skf') consists of two main blocks:

- The data block (the first part of the .skf files) and

- The documentation (second part, starting with the XML-tag `<Documentation>`).

The second part is currently not yet parsed by the DFTB+ code, but we plan to implement this feature in the future, in order to test compatibility between requested Slater-Koster files at run-time.

2 Format of the data block

The data block contains the data necessary to calculate the two center interactions. It has basically two parts:

- Header data (including an optional polynomial repulsive interaction) followed by integral tables describing the Hamiltonian and overlap matrix elements on an equidistant grid.

- Spline representation of the repulsive interaction (optional).

Below the description of the individual parts follows. The format is line based. Numbers representing physical quantities are given in atomic units (with Hartree being the energy unit) unless explicitly noted otherwise.

2.1 Header and integral tables

There are four different possible formats for the header of an SK-file. If the first character of the first line is '@', then the header and the integral table follows the extended format, allowing angular momenta up to f. Otherwise only angular momenta up to d are contained (simple format). For both formats, the headers differ for the hetero-nuclear and the homo-nuclear case.

2.1.1 Homo-nuclear case, simple format

Line 1:

```
gridDist nGridPoints
```

`gridDist` being the distance between the grid points of the integral table, and `nGridPoints` being the number of points in the table.

Line 2:

```
Ed Ep Es SPE Ud Up Us fd fp fs
```

`Ed`, `Ep` and `Es` are the on-site energies for the angular momenta d, p and s for the given atom. The field `SPE` is read but not interpreted by DFTB+ (was spin polarisation error for calculating formation energies in earlier DFTB implementations). `Ud`, `Up`, `Us` are the Hubbard U values for the appropriate angular momenta, and `fd`, `fp`, `fs` are the occupations (for the neutral atom) in the ground state.

Line 3:

```
mass c2 c3 c4 c5 c6 c7 c8 c9 rcut d1 d2 d3 d4 d5 d6 d7 d8 d9 d10
```

where `mass` is the mass of the given atom in atomic mass units (!), `c2`, ..., `c9` and `rcut` are the polynomial coefficients and the cutoff radius of the repulsive interaction (can be zero, if the repulsive is described by splines). The other numbers are only placeholders and can have arbitrary values. The polynomial repulsive is calculated as

$$\sum_{i=2}^{9} c_i (r_{\text{cut}} - r)^i. \tag{1}$$

Lines 4 to $(4 + \text{nGridPoints} - 2)$:

```
Hdd0 Hdd1 Hdd2 Hpd0 Hpd1 Hpp0 Hpp1 Hsd0 Hsp0 Hss0 Sdd0 Sdd1 Sdd2 Spd0 Spd1
Spp0 Spp1 Ssd0 Ssp0 Sss0
```

Integral table containing the DFTB Hamiltonian and the overlap matrix elements for the two center interactions dd^σ, dd^π, dd^δ, pd^σ, pd^π, pp^σ, pp^π, sd^σ, sp^σ and ss^σ between the atomic orbitals. The first line of this block corresponds to the distance `gridDist` ($|\mathbf{r}_0|$) between the atoms, for every following line the distance is increased by `gridDist`. The Hamiltonian matrix element is

$$\left\langle \phi_\mu(\mathbf{r}) \left| -\frac{1}{2}\nabla^2 + v_{\text{eff}}[n^\alpha(\mathbf{r})] + v_{\text{eff}}[n^\beta(\mathbf{r} - \mathbf{r}_0)] \right| \phi_\nu(\mathbf{r} - \mathbf{r}_0) \right\rangle \qquad \mu \in \alpha, \nu \in \beta \tag{2}$$

$$\left\langle \phi_\mu(\mathbf{r}) \left| -\frac{1}{2}\nabla^2 + v_{\text{eff}}[n^\alpha(\mathbf{r}) + n^\beta(\mathbf{r} - \mathbf{r}_0)] \right| \phi_\nu(\mathbf{r} - \mathbf{r}_0) \right\rangle \qquad \mu \in \alpha, \nu \in \beta \tag{3}$$

for the potential and the density superposition case, respectively. n^α and n^β are the atomic densities, v_{eff} is the effective potential. The overlap is

$$\langle \phi_\mu(\mathbf{r}) \,|\, \phi_\nu(\mathbf{r} - \mathbf{r}_0) \rangle \qquad \mu \in \alpha, \nu \in \beta \tag{4}$$

For both types of integrals, the direction of $\mathbf{r}_0$ is chosen to align the relevant orbitals μ and ν in the appropriate orientation for σ, π, δ, etc. bonding. The angular dependent part of the atomic orbitals is of tesseral harmonic form to be compatible with the Slater-Koster transformations.

2.1.2 Homo-nuclear case, extended format

Line 1: Comment line, starts with @ as first character.
Line 2: Identical with line 1 in the simple format.

Line 3:

```
Ef Ed Ep Es SPE Uf Ud Up Us ff fd fp fs
```

where `Ef`, `Ed`, `Ep` and `Es` are the on-site energies for the angular momenta f, d, p and s for the given atom. The field `SPE` is read but not interpreted by DFTB+ (was spin polarisation error for calculating formation energies in earlier DFTB implementations). `Uf`, `Ud`, `Up`, `Us` are the Hubbard U values for the appropriate angular momenta, and `ff`, `fd`, `fp` and `fs` are the occupations (for the neutral atom).

Line 4: Identical with line 3 in the simple format.

Lines 5 to $(5 + \texttt{nGridPoints} - 2)$:

```
Hff0 Hff1 Hff2 Hff3 Hdf0 Hdf1 Hdf2 Hdd0 Hdd1 Hdd2 Hpf0 Hpf1 Hpd0 Hpd1
Hpp0 Hpp1 Hsf0 Hsd0 Hsp0 Hss0  Sff0 Sff1 Sff2 Sff3 Sdf0 Sdf1 Sdf2 Sdd0
Sdd1 Sdd2  Spf0 Spf1 Spd0 Spd1 Spp0 Spp1 Ssf0 Ssd0 Ssp0 Sss0
```

Integral table containing the Hamiltonian matrix elements and the overlaps for the two center interactions $ff\sigma$, $ff\pi$, $ff\delta$ $ff\phi$, $df\sigma$, $df\pi$, $df\delta$, $dd\sigma$, $dd\pi$, $dd\delta$, $pf\sigma$, $pf\pi$, $pd\sigma$, $pd\pi$, $pp\sigma$, $pp\pi$, $sf\sigma$, $sd\sigma$, $sp\sigma$, $ss\sigma$. The first line of this block corresponds to the distance `gridDist` between the atoms, for every following line the distance is increased by `gridDist`. (The angular dependent part of the atomic orbitals in the integrals is assumed being described by tesseral harmonics.)

2.1.3 Hetero-nuclear case, simple format

Line 1: The same as line 1 in the homo-nuclear case.

Line 2: The same as line 3 in the homo-nuclear case, however the `mass` field is just a placeholder.

Lines 3 to $(3 + \texttt{nGridPoints} - 2)$: The same as lines 4 to $(4 + \texttt{nGridPoints} - 2)$ in the homo-nuclear case.

2.1.4 Hetero-nuclear case, extended format

Line 1: Identical to line 1 in the homo-nuclear case.

Lines 2 to 3: Identical to lines 1 to 2 in the simple format (hetero-nuclear case).

Lines 4 to (4 + nGridPoints - 2): Identical to lines 5 to (5 + nGridPoints - 2) in the homo-nuclear case.

2.2 Spline repulsive

This part describes the repulsive interaction via splines. It is optional, as the header contains coefficients for a polynomial description which can be used instead of the splines. The spline block (if present) contains following lines:

Line 1:

Spline

Simple line with the string 'Spline' indicating the start of the block with the spline repulsive.

Line 2:

nInt cutoff

with nInt being the number of (subsequent) intervals being described by various cubic splines and cutoff the cutoff of the repulsive interaction.

Line 3:

a1 a2 a3

Coefficients to describe the exponential part of the repulsive (which is applied if the atoms are closer as the starting distance of the first spline). The repulsive in that region is described by the exponential expression

$$e^{-a_1 r + a_2} + a_3 \qquad (5)$$

with r being the distance between the atoms.

Lines 4 to 4 + nInt - 2:

start end c0 c1 c2 c3

with start (r_0) and end describing the bounds of the distance range, on which the current spline describes the repulsive interaction as

$$c_0 + c_1(r - r_0) + c_2(r - r_0)^2 + c_3(r - r_0)^3. \qquad (6)$$

Please note, that end is read but not interpreted by DFTB+, as the end of an interval is taken to be equal to the start of the next interval. (Anything else would be illogical anyway.)

Nevertheless `end` should be specified in each line correctly, as other DFTB implementations may depend on it.

Line 4 +`nInt` - 1:

`start end c0 c1 c2 c3 c4 c5`

with `start` (r_0) and `end` describing the bounds of the distance range, on which the last spline describes the repulsive interaction as

$$c_0 + c_1(r - r_0) + c_2(r - r_0)^2 + c_3(r - r_0)^3 + c_4(r - r_0)^4 + c_5(r - r_0)^5. \tag{7}$$

Please note, that `end` is read but not interpreted by DFTB+, as the end of the last interval is taken to be equal to `cutoff`. (Anything else would be illogical anyway.) Nevertheless `end` should be specified in each line correctly, as other DFTB implementations may depend on it.