SPARC - SQ

Spectral Quadrature method

User guide

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Comments

The code will fail with the following options and the related input options are listed.

- Polarized calculation: `SPIN_TYP`.
- K-point calculation: `KPOINT_GRID`, `KPOINT_SHIFT`.
- Dirichlet boundary condition in any direction: `BC`
- Define number of states/orbitals: `NSTATES`
- CS and SQ3 method: `CS_FLAG, SQ3_FLAG`
- Hybrid functionals: `EXCHANGE_CORRELATION`
- Print eigenvalues into file: `PRINT_EIGEN`

Input file options

SQ

SQ_FLAG | SQ_TYPE_DM | SQ_GAUSS_MEM | SQ_NPL_C | SQ_NPL_G | SQ_RCUT | SQ_FAC_G2C | SQ_TOL_OCC | SQ_EIGSHIFT_FLAG| SQ_EIGSHIFT

SQ

SQ_FLAG

Type

Integer

Unit

No unit

Default

0

Example

```
SQ_FLAG: 1
```

Description

Flag to turn on SQ method

Remark

SQ method can not be turned on simultaneously with CS, SQ3, hybrid functionals.

SQ_TYPE_DM

Type

String

Unit

No unit

Default

GAUSS

Example

SQ_TYPE_DM: CC

Description

Flag to choose type of quadrature for density matrix. Available options are Gauss (GAUSS) and Clenshaw-Curtis (CC).

SQ_GAUSS_MEM

Type

String

Unit

No unit

Default

LOW

Example

SQ_GAUSS_MEM: HIGH

Description

Flag for memory option when using Gauss quadrature for density matrix.

SQ_NPL_C

Type

Integer

Unit

No unit

Default

SQ_NPL_G × SQ_FAC_G2C

Example

SQ_NPL_C: 24

Description

Degree of polynomial for Clenshaw Curtis in forces and stress.

SQ_NPL_G

Type

Integer

Unit

No unit

Default

None

Example

SQ_NPL_G: 24

Description

Degree of polynomial for Gauss Quadrature.

Remark

SQ_NPL_G must be specified if SQ is turned on.

SQ_RCUT

Type

Double

Unit

Bohr

Default

None

Example

SQ_RCUT: 2.0

Description

Truncation or localization radius

Remark

SQ_RCUT must be specified if SQ is turned on.

SQ_FAC_G2C

Type

Double

Unit

No unit

Default

2.0

Example

SQ_FAC_G2C: 3.0

Description

SQ_NPL_C = SQ_FAC_G2C × SQ_NPL_G. Used if SQ_NPL_C is not specified.

SQ_TOL_OCC

Type

Double

Unit

No unit

Default

10^{-6}

Example

SQ_TOL_OCC: 1E-5

Description

Tolerance for occupation corresponding to maximum eigenvalue.

SQ_EIGSHIFT_FLAG

Type

Integer

Unit

No unit

Default

0

Example

```
SQ_EIGSHIFT_FLAG: 1
```

Description

Flag for choosing to use minmax eigenvalues of Gauss for Clenshaw Curtis in forces/stress after shifting by eigshift.

SQ_EIGSHIFT

Type

Double

Unit

Percent

Default

5

Example

SQ_EIGSHIFT: 10

Description

Percentage shift in eigenspectrum.