SPARC - SQ

Spectral Quadrature method

User guide

Material Physics & Mechanics Group
PI: Phanish Suryanarayana
Main Developers: Xin Jing, Abhiraj Sharma, Phanisri P. Pratapa
Collaborators: J.E. Pask (LLNL)
Georgia Institute of Technology

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
- Hybrid functionals: EXCHANGE_CORRELATION
- Print eigenvalues into file: PRINT_EIGEN

Input file options

Spectral Quadrature

`SQ_FLAG` | `SQ_RCUT` | `SQ_NPL_G` | `SQ_GAUSS_MEM` | `SQ_TOL_OCC` |
`NP_DOMAIN_SQ_PARAL`

Spectral Quadrature

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_RCUT

Type	Unit
Double	Bohr

Default	Example
None	`SQ_RCUT: 2.0`

Description

Truncation or localization radius

Remark

`SQ_RCUT` must be specified if SQ is turned on.

SQ_NPL_G

Type	Unit
Integer	No unit

Default	Example
None	SQ_NPL_G: 24

Description

Degree of polynomial for Gauss Quadrature.

Remark

SQ_NPL_G must be specified if SQ is turned on.

SQ_GAUSS_MEM

Type	Unit
String	No unit

Default	Example
LOW	SQ_GAUSS_MEM: HIGH

Description

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

SQ_TOL_OCC

Type	Unit
Double	No unit

Default	Example
10^{-6}	SQ_TOL_OCC: 1E-5

Description

Tolerance for occupation corresponding to maximum eigenvalue.

NP_DOMAIN_SQ_PARAL

Type
Integer

Unit
No unit

Default
Automatically optimized

Example
NP_DOMAIN_SQ_PARAL: 3 3 2

Description
Dimensions of the 3D Cartesian topology for SQ method.

Remark
This option is for development purpose. It's better to let SPARC choose the parallization parameters in practice.