SPARC-cyclix

User guide

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Contributors

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Citation

If you publish work using/regarding SPARC-cyclix, please cite the following article, in addition to SPARC citations:

- https://doi.org/10.1103/PhysRevB.103.035101
- Additional references for initial developments: https://doi.org/10.1016/j.jmps.2016.08.007, https://doi.org/10.1103/PhysRevB.100.125143

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Input file options

Input file options for SPARC-cyclix, in addition to SPARC:

Cyclix

TWIST_ANGLE | BC | CELL | COORD | COORD_FRAC | EXCHANGE_CORRELATION | KPOINT_GRID |

TWIST_ANGLE

Type

Double

Unit

rad/Bohr

Default

0

Example

`TWIST_ANGLE: 0.0045`

Description

External twist per unit length applied on the nanotube.

Remark

If using helical symmetry (D C H), we also have to add the intrinsic twist.

BC

Type

Character

Unit

No Unit

Default

None

Example

BC: D C P

Description

A set of three whitespace delimited characters specifying the boundary conditions in the lattice vector directions, respectively. P represents periodic boundary conditions, D represents Dirichlet boundary conditions, C represents cyclic boundary conditions and H represents helical boundary conditions.

BC

Remark

`BC: D C P` and `BC: D C H` are the cyclix cases where the former uses only cyclic boundary condition and latter uses both cyclic and helical boundary conditions.

CELL

Type

Double

Unit

Bohr

Default

None

Example

`CELL: 30.3498 0.2991 3.1359`

Description

A set of three whitespace delimited values specifying the cell lengths in the radial, angular and periodic/helical directions, respectively.

Remark

Angular direction length is equal to $2\pi/\Gamma$, where Γ is the group order in the cyclic direction.

COORD

Type

Double

Unit

Bohr

Default

None

Example

```
COORD:
0 0 0
2.5 2.5 2.5
```

Description

The Cartesian coordinates of atoms of a ATOM_TYPE specified before this variable. If the coordinates are outside the fundamental domain (see CELL) in the periodic and cyclic/helical directions (see BC), it will be automatically mapped back to the domain.

COORD

Remark

For a system with different types of atoms, one has to specify the coordinates for every ATOM_TYPE. One can also specify the coordinates of the atoms using COORD_FRAC.

COORD_FRAC

Type

Double

Unit

None

Default

None

Example

```
COORD_FRAC:
0 0 0
2.1 0.5 0.5
```

Description

The fractional coordinates of atoms of a ATOM_TYPE specified before this variable. COORD_FRAC$(i, j) \times$ CELL$(j), (j = 1, 2, 3)$ gives the coordinate of the i^{th} atom along the j^{th} direction. $j = 1$ is along radial, $j = 2$ is along angular and $j = 3$ is along periodic/helical direction.

COORD_FRAC

Remark

For a system with different types of atoms, one has to specify the coordinates for every ATOM_TYPE. One can also specify the coordinates of the atoms using COORD.

EXCHANGE_CORRELATION

Type

String

Unit

No unit

Default

No Default

Example

```
EXCHANGE_CORRELATION:
LDA_PW
```

Description

Choice of exchange-correlation functional. Options are `LDA_PW` (Perdew-Wang LDA), `LDA_PZ` (Purdew-Zunger LDA) and `GGA_PBE` (PBE GGA)

EXCHANGE_CORRELATION

Remark

For spin-polarized calculation (SPIN_TYP = 1), LDA_PW (Perdew-Wang LDA) and GGA_PBE (PBE GGA) are available.

KPOINT_GRID

Type

Integer array

Unit

No unit

Default

1 1 1

Example

`KPOINT_GRID: 1 5 10`

Description

Number of k-points in each direction of the Monkhorst-Pack grid for Brillouin zone integration. In SPARC-cyclix, we don't have any k-points along the radial direction as it is vaccuum. The angular k-point is reffered as ν point and the periodic/helical k-point is called η point.

Remark

ν point should be an integer factor of the group order Γ.

FAQs

Q: How can SCF convergence be made better in SPARC-cyclix calculations?
A: In cases of smaller radius and finer mesh, we need to use higher Chebyshev Degree. Increasing the option CHEB_DEGREE should help with the SCF convergence.

Q: Are pseudopotentials with non-linear core corrections and relativistic effect supported by SPARC-cyclix?
A: Yes.

Q: Is non-collinear spin calculation supported by SPARC-cyclix?
A: No, currently we only have the collinear spin calculations available in SPARC-cyclix.