SPARC

PBEq convolutional exchange correlation functional

Documentation

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Acknowledgements

- U.S. Department of Energy, Basic Energy Sciences, Computational Chemical Sciences Program: DESC0019410
- Partnership for an Advanced Computing Environment (PACE): 1828187

Comments

Key notes:

- Input and output files for molecules, metals and chemisorption systems for PBEq15 (best functional) are provided in the GitHub repository.
- Force and stress calculations are not yet implemented for the convolutional PBEq functional.
- MCSH stands for Maxwell Cartesian Spherical Harmonics.
- Additional term in exchange potential calculation arising due to monopole dependence is neglected, by default. The source code needs to be changed directly if the user wants to test the functional for small `M_VAL`.

Comments

This is an experimental functional, and only the following arguments can be changed:

- `MCSH_MAX_R`: Maximum radial cut-off for MCSH expansion
- `MCSH_R_STEPSIZE`: Step-size for radial cut-off for MCSH expansion
- `N_VAL`: Value of parameter n that determines α in PBEq functional

Note that the `PBEq` functional is not dependent on `MCSH_R_STEPSIZE`, hence it can be set to any value. This option is required in the input file for correct initialization of descriptor calculation.

Comments

The following arguments cannot be changed:

- `MCSH_MAX_ORDER`: Order of MCSH should be set to 0
- `MCSH_RADIAL_TYPE`: Type of radial basis function for MCSH expansion should be set to 1
- `EXCHANGE_CORRELATION`: Exchange correlation functional should be set to `GGA_CONV_PBE_MULTIPOLE`
- `M_VAL`: Value of parameter m should be set to a large value (e.g. 10^6) because additional term in exchange potential is neglected
- `RELAX_FLAG`: Structural relaxation should be turned off

They are included in the documentation for completeness.

Input file options

Convolutional PBEq

EXCHANGE_CORRELATION | MCSH_RADIAL_TYPE | MCSH_R_STEPSIZE | MCSH_MAX_ORDER | MCSH_MAX_R | N_VAL | M_VAL

Convolutional PBEq

EXCHANGE_CORRELATION

Type

String

Unit

No unit

Default

No Default

Example

```
EXCHANGE_CORRELATION:
GGA_CONV_PBE_MULTIPOLE
```

Description

Flag to use for PBEq convolutional exchange correlation functional.

Remark

All the other options in this documentation should be specified if EXCHANGE_CORRELATION is set to GGA_CONV_PBE_MULTIPOLE.

MCSH_RADIAL_TYPE

Type

Integer

Unit

No unit

Default

1

Example

```
MCSH_RADIAL_TYPE: 1
```

Description

Type of radial basis function for multipole expansion. The convolutional PBEq is only implemented for `MCSH_RADIAL_TYPE = 1` which denotes heaviside step function.

Remark

`MCSH_RADIAL_TYPE = 2` cannot be used with convolutional PBEq.

MCSH_R_STEPSIZE

Type

Double

Unit

Bohr

Default

3.0

Example

```
MCSH_R_STEPSIZE: 3.0
```

Description

Cut-off radius for MCSH expansion.

MCSH_MAX_ORDER

Type

Integer

Unit

No unit

Default

0

Example

MCSH_MAX_ORDER: 0

Description

Maximum order of MCSH expansion.

Remark

MCSH_MAX_ORDER should be equal to 0 for PBEq functional. It is currently not developed for higher orders of MCSH.

MCSH_MAX_R

Type

Double

Unit

Bohr

Default

3.0

Example

MCSH_MAX_R: 3.0

Description

MCSH_MAX_R is the maximum radius for MCSH expansion.

N_VAL

Type

Double

Unit

No unit

Default

0.0

Example

N_VAL: 15.0

Description

The value of parameter n that determines the spatially-resolved α in the PBEq functional.

Remark

For the best functional inPBEq class of functionals, N_VAL is set to 15.0.

M_VAL

Type

Double

Unit

No unit

Default

0.0

Example

M_VAL: 1000000.0

Description

The value of parameter m that determines the spatially-resolved α in the PBEq functional.

Remark

For the best functional in PBEq class of functionals, M_VAL is set to 1000000.0 and the additional terms in exchange potential are neglected.