cDFT Keywords

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Intermediate Keywords

Keyword	Type	Descriptions
CDFT_ATOM_CHARGE	Logical	Activate atom charge-constrained constrained-DFT mode
CDFT_ATOM_SPIN	Logical	Activate atom magnetic-moment-constrained DFT mode
CDFT_CG_MAX	Integer	Reset frequency for constraining-potential (Uq/s) conjugate gradient optimisation
CDFT_CG_MAX_STEP	Integer	Maximum length of trial step for constraining-potential (Uq/s) optimisation line search
CDFT_CG_THRESHOLD	Real	Convergence threshold for constraining-potential (Uq/s) RMS gradient
CDFT_CG_TYPE	Text	Variant of conjugate gradient algorithm to use for constraining-potential (Uq/s) optimisation
CDFT_CHARGE_ACCEPTOR_TARGET	Real	Targeted e-population for charge-constrained acceptor-group
CDFT_CHARGE_DONOR_TARGET	Real	Targeted e-population for charge-constrained donor-group
CDFT_CONTINUATION	Logical	Continue a previous optimisation of the cDFT constraining potentials
CDFT_GROUP_CHARGE_ACCEPTOR	Logical	Activate acceptor-group charge-constrained DFT mode
CDFT_GROUP_CHARGE_DIFF	Logical	Activate group charge-difference (acceptor-donor) constrained DFT mode
CDFT_GROUP_CHARGE_DIFF_TARGET	Real	Targeted (acceptor-donor) e-population difference for group charge-difference constrained-DFT
CDFT_GROUP_CHARGE_DONOR	Logical	Activate donor-group charge-constrained DFT mode
CDFT_GROUP_CHARGE_DOWN_ONLY	Logical	Constrain only SPIN-DOWN channel in group_charge_acceptor/donor and group_charge_diff modes
CDFT_GROUP_CHARGE_UP_ONLY	Logical	Constrain only SPIN-UP channel in group_charge_acceptor/donor and group_charge_diff modes

CDFT_GROUP_SPIN_ACCEPTOR	Logical	Activate acceptor-group magnetic-moment-constrained DFT mode
CDFT_GROUP_SPIN_DIFF	Logical	Activate group magnetic-moment-difference (acceptor-donor) constrained DFT mode
CDFT_GROUP_SPIN_DIFF_TARGET	Real	Targeted (acceptor-donor) magnetic-moment difference for magnetic-moment-difference constrained-DFT
CDFT_GROUP_SPIN_DONOR	Logical	Activate donor-group magnetic-moment-constrained DFT mode
CDFT_GURU	Logical	Tell ONETEP you are a cDFT expert and do not need any help in initialising the cDFT run
CDFT_HUBBARD	Logical	Activate cDFT+U functionality
CDFT_MAX_GRAD	Real	Convergence threshold for maximum constraining-potential (Uq/s) gradient at any cDFT-site
CDFT_MULTI_PROJ	Logical	Activate “as many cDFT-projectors as NGWFs” mode
CDFT_PRINT_ALL_OCC	Logical	Print subspace occupancies for all cDFT-sites
CDFT_READ_PROJ	Logical	Read cDFT-projectors from `.tightbox_hub_proj` file
CDFT_SPIN_ACCEPTOR_TARGET	Real	Targeted magnetic-moment for magnetic-moment-constrained acceptor-group
CDFT_SPIN_DONOR_TARGET	Real	Targeted magnetic-moment for magnetic-moment-constrained donor-group
CDFT_TRIAL_LENGTH	Real	Set initial trial length for first step of cDFT conjugate gradients optimisation
CI_CDFT	Logical	Perform a Configuration Interatcion constrained-DFT simulation [to be converted into a TASK…]
CI_CDFT_NUM_CONF	Integer	Number of cDFT configurations for CI-cDFT simulation
CONSTRAINED_DFT	Block	Activate constrained-DFT functionality
MAXIT_CDFT_U_CG	Integer	Maximum number of constraining-potential (Uq/s) conjugate gradient iterations

CDFT_ATOM_CHARGE

Syntax: `CDFT_ATOM_CHARGE [Logical]`

Description: Activate atom charge-constrained-DFT mode. This mode is incompatible with any other cDFT-mode.

Default: `False`

Example: `CDFT_ATOM_CHARGE T`

CDFT_ATOM_SPIN

Syntax: `CDFT_ATOM_SPIN [Logical]`

Description: Activate atom magnetic-moment-constrained-DFT mode. This mode is incompatible with any other cDFT-mode.

Default: `False`

Example: `CDFT_ATOM_SPIN T`

CDFT_CG_MAX

Syntax: `CDFT_CG_MAX [Real]`

Description: Specifies the maximum number of constraining potential (Uq/s) conjugate gradient iterations between resets.

Default: Number of independent Uq/s for `cdft_guru=F`

Example:
```
CDFT_CG_MAX 1  #Perform steepest descents optimisation
```

CDFT_CG_MAX_STEP

Syntax: `CDFT_CG_MAX_STEP [Real]`

Description: Maximum length of trial step for the constraining potential (Uq/s) optimisation line search.

Default: `50.0`

Example: `CDFT_CG_MAX_STEP 10.0`

CDFT_CG_THRESHOLD

Syntax: `CDFT_CG_THRESHOLD [Real]`

Description: Specifies the convergence threshold for the RMS gradient of the constraining potentials (Uq/s).

Default: `1.0E-3`

Example: `CDFT_CG_THRESHOLD 0.01`

CDFT_CG_TYPE

Syntax: `CDFT_CG_TYPE [Text]`

Description: Specifies the variant of the conjugate gradients algorithm used for the optimization of the constraining potentials (Uq/s), currently either `NGWF_FLETCHER` for Fletcher-Reeves or `NGWF_POLAK` for Polak-Ribiere.

Default: `NGWF_FLETCHER`

Example: `CDFT_CG_TYPE NGWF_POLAK`

CDFT_CHARGE_ACCEPTOR_TARGET

Syntax: `CDFT_CHARGE_ACCEPTOR_TARGET [Real]`

Description: Targeted acceptor-group electron population for acceptor-group charge-constrained-DFT mode [`CDFT_GROUP_CHARGE_ACCEPTOR=T`].

Default: `0.`

Example: `CDFT_CHARGE_ACCEPTOR_TARGET 17 #Constrain Nup+Ndown=17 e in subspace`

CDFT_CHARGE_DONOR_TARGET

Syntax: `CDFT_CHARGE_DONOR_TARGET [Real]`

Description: Targeted donor-group electron population for donor-group charge-constrained-DFT mode [`CDFT_GROUP_CHARGE_DONOR=T`].

Default: `0.`

Example: `CDFT_CHARGE_DONOR_TARGET 17 #Constrain Nup+Ndown=17 e in subspace`

CDFT_CONTINUATION

Syntax: `CDFT_CONTINUATION [Logical]`

Description: Continue a constraining potential (Uq/s) optimisation from a previous run using the `.cdft` file with the latest cDFT-potentials. `CDFT_CONTINUATION=T` allows also to perform single-point cDFT runs (`MAXIT_CDFT_U_CG=0`) reading atom-specific constraining potentials from `.cdft` file (instead of species-specific ones from the `CONSTRAINED_DFT` block). For `cdft_continuation=T`, the constraining potentials (Uq/s) are read from the `.cdft` file no matter the setting of `cdft_guru`.

Default: `False`

Example: `CDFT_CONTINUATION T`

CDFT_GROUP_CHARGE_ACCEPTOR

Syntax: CDFT_GROUP_CHARGE_ACCEPTOR [Logical]

Description: Activate acceptor-group charge-constrained-DFT mode. This mode is compatible with CDFT_GROUP_CHARGE_DONOR and CDFT_GROUP_SPIN_ACCEPTOR/DONOR cDFT-modes, and incompatible with CDFT_ATOM_CHARGE/SPIN and CDFT_GROUP_CHARGE/SPIN_DIFF cDFT modes.

Default: False

Example: CDFT_GROUP_CHARGE_ACCEPTOR T

CDFT_GROUP_CHARGE_DIFF

Syntax: CDFT_GROUP_CHARGE_DIFF [Logical]

Description: Activate group charge-difference constrained-DFT mode. This mode is compatible with CDFT_GROUP_SPIN_DIFF cDFT mode only. Thus, it is incompatible with any other CDFT_ATOM_CHARGE/SPIN and CDFT_GROUP_CHARGE/SPIN_ACCEPTOR/DONOR cDFT modes.

Default: False

Example: CDFT_GROUP_CHARGE_DIFF T

CDFT_GROUP_CHARGE_DIFF_TARGET

Syntax: CDFT_CHARGE_DIFF_TARGET [Real]

Description: Targeted electron population difference between acceptor and donor group for -group charge-difference constrained-DFT mode [CDFT_GROUP_CHARGE_DIFF=T].

Default: 0.

Example: CDFT_CHARGE_ACCEPTOR_TARGET 2
#Constrain [Nup+Ndown]_ACC - [Nup+Ndown]_DON to 2 e.

CDFT_GROUP_CHARGE_DONOR

Syntax: CDFT_GROUP_CHARGE_DONOR [Logical]

Description: Activate donor-group charge-constrained-DFT mode. This mode is compatible with CDFT_GROUP_CHARGE_ACCEPTOR and CDFT_GROUP_SPIN_ACCEPTOR/DONOR cDFT-modes, and incompatible with CDFT_ATOM_CHARGE/SPIN and CDFT_GROUP_CHARGE/SPIN_DIFF cDFT modes.

Default: False

Example: CDFT_GROUP_CHARGE_DONOR T

CDFT_GROUP_CHARGE_DOWN_ONLY

Syntax: CDFT_GROUP_CHARGE_DOWN_ONLY [Logical]

Description: Constrain only SPIN-DOWN channel in CDFT_GROUP_CHARGE_ACCEPTOR, CDFT_GROUP_CHARGE_DONOR and CDFT_GROUP_CHARGE_DIFF modes. To avoid disaster, make sure the specified CDFT_CHARGE_ACCEPTOR/DONOR_TARGET or CDFT_CHARGE_DIFF_TARGET keywords are consistent with the fact only one spin channel is being constrained. This functionality is NOT compatible with CDFT_GROUP_CHARGE_UP_ONLY, CDFT_ATOM_CHARGE/SPIN, and CDFT_GROUP_SPIN_ACCEPTOR/DONOR and CDFT_GROUP_SPIN_DIFF cDFT modes.

Default: False

Example: CDFT_GROUP_CHARGE_DOWN_ONLY T

CDFT_GROUP_CHARGE_UP_ONLY

Syntax: CDFT_GROUP_CHARGE_UP_ONLY [Logical]

Description: Constrain only SPIN-UP channel in CDFT_GROUP_CHARGE_ACCEPTOR, CDFT_GROUP_CHARGE_DONOR and CDFT_GROUP_CHARGE_DIFF modes. To avoid disaster, make sure the specified CDFT_CHARGE_ACCEPTOR/DONOR_TARGET or CDFT_CHARGE_DIFF_TARGET keywords are consistent with the fact only one spin channel is being constrained. This functionality is NOT compatible with CDFT_GROUP_CHARGE_DOWN_ONLY, CDFT_ATOM_CHARGE/SPIN, and CDFT_GROUP_SPIN_ACCEPTOR/DONOR and CDFT_GROUP_SPIN_DIFF cDFT modes.

Default: False

Example: CDFT_GROUP_CHARGE_UP_ONLY T

CDFT_GROUP_SPIN_ACCEPTOR

Syntax: CDFT_GROUP_SPIN_ACCEPTOR [Logical]

Description: Activate acceptor-group magnetic-moment constrained-DFT mode. This mode is compatible with CDFT_GROUP_SPIN_DONOR and CDFT_GROUP_CHARGE_ACCEPTOR/DONOR cDFT-modes, and incompatible with CDFT_ATOM_CHARGE/SPIN and CDFT_GROUP_CHARGE/SPIN_DIFF cDFT modes.

Default: False

Example: CDFT_GROUP_SPIN_ACCEPTOR T

CDFT_GROUP_SPIN_DIFF

Syntax: CDFT_GROUP_SPIN_DIFF [Logical]

Description: Activate group magnetic-moment-difference constrained-DFT mode. This mode is compatible with CDFT_GROUP_CHARGE_DIFF cDFT mode only. Thus, it is incompatible with any other CDFT_ATOM_CHARGE/SPIN and CDFT_GROUP_CHARGE/SPIN_ACCEPTOR/DONOR cDFT modes.

Default: False

Example: CDFT_GROUP_CHARGE_DIFF T

CDFT_GROUP_SPIN_DIFF_TARGET

Syntax: CDFT_SPIN_DIFF_TARGET [Real]

Description: Targeted magnetic-moment difference between acceptor and donor group for group magnetic-moment-difference constrained-DFT mode [CDFT_GROUP_SPIN_DIFF=T].

Default: 0.

Example: CDFT_CHARGE_ACCEPTOR_TARGET 2
#Constrain [Nup-Ndown]_ACC - [Nup-Ndown]_DON to 2 e.

CDFT_GROUP_SPIN_DONOR

Syntax: CDFT_GROUP_SPIN_DONOR [Logical]

Description: Activate donor-group magnetic-moment constrained-DFT mode. This mode is compatible with CDFT_GROUP_SPIN_ACCEPTOR and CDFT_GROUP_CHARGE_ACCEPTOR/DONOR cDFT-modes, and incompatible with CDFT_ATOM_CHARGE/SPIN and CDFT_GROUP_CHARGE/SPIN_DIFF cDFT modes.

Default: False

Example: CDFT_GROUP_SPIN_DONOR T

CDFT_GURU

Syntax: CDFT_GURU [Logical]

Description: Tell ONETEP you are a cDFT-expert and prevent it from initialising the active |Uq/s| to failsafe value of 1 eV overwriting the values entered in the %block constrained_dft (Uq/s).

Default: False

Example: CDFT_GURU T

CDFT_HUBBARD

Syntax: `CDFT_HUBBARD [Logical]`

Description: Activate the constrained-DFT+U functionality. It requires specifications of a positive value for the Hubbard correction (Uh) in the `CONSTRAINED_DFT Block.`

Default: `False`

Example: `CDFT_HUBBARD T`

CDFT_MAX_GRAD

Syntax: `CDFT_MAX_GRAD [Real]`

Description: Specifies the convergence threshold for the maximum value of the constraining-potential (Uq/s) gradient at any cDFT-site

Default: `1.0E-3`

Example: `CDFT_MAX_GRAD 0.01`

CDFT_MULTI_PROJ

Syntax: `CDFT_MULTI_PROJ [Logical]`

Description: Activate the “as many cDFT-projectors as NGWFs” cDFT-mode. In this mode, the number of cDFT-projectors for a given cDFT-atom equals the number of NWGFs for that atom as specified in the `%block species`. Both the cDFT-projectors and the NGWFs are localised within spheres of the same radius. When activated, this mode overwrites the L-projectors and Z-projectors settings in `%block constrained_dft`, and the cDFT-projectors are built according to the settings in `%block species_atomic_set` for that atom=cDFT-site.

Default: `False`

Example: `CDFT_MULTI_PROJ T`

CDFT_PRINT_ALL_OCC

Syntax: `CDFT_PRINT_ALL_OCC [Logical]`

Description: Print detailed information of occupancies for al the cDFT-sites, for `OUTPUT_DETAIL = VERBOSE`.

Default: `False`

Example: `CDFT_PRINT_ALL_OCC T`

CDFT_READ_PROJ

Syntax: `CDFT_READ_PROJ [Logical]`

Description: Read cDFT-projectors from `.tightbox_hub_proj` file. Activation of this keyword overwrites any Z-projector setting in `%block constrained_dft`. It also makes not necessary to set `hubbard_proj_mixing<0` to have `task=HUBBARDSCF` runs with projectors read in from file.

Default: `False`

Example: `CDFT_READ_PROJ T`

CDFT_SPIN_ACCEPTOR_TARGET

Syntax: `CDFT_SPIN_ACCEPTOR_TARGET [Real]`

Description: Targeted group magnetic-moment for acceptor-group magnetic-moment constrained-DFT mode [`CDFT_GROUP_SPIN_ACCEPTOR=T`].

Default: `0.`

Example: `CDFT_SPIN_ACCEPTOR_TARGET -2 #Constrain Nup-Ndown=-2 in subspace`

CDFT_SPIN_DONOR_TARGET

Syntax: `CDFT_SPIN_DONOR_TARGET [Real]`

Description: Targeted group magnetic-moment for donor-group magnetic-moment constrained-DFT mode [`CDFT_GROUP_SPIN_DONOR=T`].

Default: `0.`

Example: `CDFT_SPIN_DONOR_TARGET -2 #Constrain Nup-Ndown=-2 in subspace`

CDFT_TRIAL_LENGTH

Syntax: `CDFT_TRIAl_LENGTH [Real]`

Description: Specifies initial trial length for first step of constraining-potential (Uq/s) conjugate gradients optimisation.

Default: `0.1`

Example: `CDFT_TRIAL_LENGTH 1.0`

CI_CDFT

Syntax: `CI_CDFT [Logical]`

Description: Perform a Configuration Interaction calculation based on constrained-DFT configurations.

Default: `False`

Example: `CI_CDFT T`

CI_CDFT_NUM_CONF

Syntax: CDFT_MAX_GRAD [Integer]

Description: Specifies the number of constrained-DFT configuration available for a CI_CDFT=T simulation

Default: 0

Example: CI_CDFT_NUM_CONF 4

CONSTRAINED_DFT

Syntax: CONSTRAINED_DFT [Block]

Syntax:
```
%BLOCK CONSTRAINED_DFT
S1 L1 Z1 Uh1 Uq1(UP) Uq1(DOWN) Us1 N1(UP) N1(DOWN) [N1(UP)-N1(DOWN)]
S2 L2 Z2 Uh2 Uq2(UP) Uq2(DOWN) Us2 N2(UP) N2(DOWN) [N2(UP)-N2(DOWN)]
. . . . .
. . . . .
SM LM ZM UhM UqM(UP) UqM(DOWN) UsM NM(UP) NM(DOWN) [NM(UP)-NM(DOWN)]
%ENDBLOCK CONSTRAINED_DFT
```

Description: Manages constrained-DFT simulations. Provided cdft_multi_proj=F, for species S and subspace of angular momentum channel L (with principal quantum number n=L+1) we apply charge spin-specific [Uq(UP), Uq(DOWN)] or magnetic-moment-specific (Us) constraining potentials (eV). For cdft_atom_charge=T, N(UP) and N(DOWN) indicate the targeted e-population for spin-channel UP and DOWN, respectively. For cdft_atom_spin=T, [N1(UP)-N1(DOWN)] indicates the targeted e-population difference (i.e. local magnetic moment). Uh indicates the optional Hubbard parameter (U, eV) to be applied for cdft_hubbard=T. An effective nuclear charge Z defines the hydrogenic orbitals spanning the subspace unless a negative value is given, e.g., Z=-10, in which case the NGWFs initial guess orbitals (numerical atomic orbitals) are used. Depending on the activated cDFT-mode, different columns of the block are used. These are:

S, L, Z, (Uh), Uq(UP), Uq(DOWN), N(UP), N(DOWN) for cdft_atom_charge=T

S, L, Z, (Uh), Us, [N(UP)-N(DOWN)] for cdft_atom_spin=T

S, L, Z, (Uh), Uq(UP), Uq(DOWN) for cdft_group_charge_acceptor=T, cdft_group_charge_donor=T, or cdft_group_charge_diff=T. In this case, Uq(UP) must be equal to Uq(DOWN). Acceptor and donor atoms are differentiated by mean of negative [Uq(UP/DOWN)<0] and positive [Uq(UP/DOWN)>0] constraining-potentials, respectively. Setting Uq=0 in the %block constrained_dft will result in the given cDFT-

atom being excluded from the list of the atoms in a given cdft_group_charge_donor/acceptor/diff group.

S, L, Z, (Uh), and Us for cdft_group_spin_acceptor=T, cdft_group_spin_donor=T, or cdft_group_spin_diff=T. In this case, Acceptor and donor atoms are differentiated by mean of negative (Us<0) and positive (Us>0) constraining-potentials, respectively. Setting Us=0 in the %block constrained_dft will result in the given cDFT-atom being excluded from the list of the atoms in a given cdft_group_spin_donor/acceptor/diff group.

cdft_group_spin_acceptor=T, cdft_group_spin_donor=T, cdft_group_charge_acceptor=T and cdft_group_charge_donor=T are all compatible one with another. Charge- and magnetic-moment acceptor- and donor-groups may or may not be the same group. Thus, besides simultaneously constraining the charge and magnetic-moment on a given group, it is also possible (by setting the appropriate sign of Uq and Us in the %block constrained_dft) to create, within the same input and system, a charge_acceptor group-A, a charge_donor group-B, a spin_acceptor group-C and a spin_donor group-C. Similar considerations apply also for simultaneous activation of group_charge_diff and group_spin_diff cDFT-modes. In sum,

Activation of cdft_group_charge_up(down)_only=T for cdft_group_charge_acceptor/donor or cdft_group_charge_diff modes leads to optimisation of the Uq potentials only for the selected spin-channel i.e. Uq(UP) only for cdft_group_charge_up_only=T, and Uq(DOWN) only for cdft_group_charge_down_only=T, leaving the other spin channel unconstrained.

For cdft_multi_proj=T the L-projector and Z-projector columns in the %block constrained_dft are read but NOT used. The cDFT-projectors are set on the basis of the %block species_atomic_set and taken as the NGWFs initial guess (numerical atomic orbital). This leads to as many cDFT-projectors as NGWFs for the cDFT-atom being used. In the current implementation, the same Uq/s is applied to all the projectors of a given cDFT-atom regardless of their principal quantum number and angular momentum.

For all the cDFT-modes, unless maxit_cdft_u_cg=0, and depending of the specific cDFT-mode, the constraining potentials (Uq, Us) will be automatically optimised. Note that, unless cdft_guru=T, the constraining potentials (Uq/s) will be initialised to 1 eV. Thus, to perform fixed-Uq/s cDFT-runs or to initialise Uq/s with values different from 1 eV (useful for low-energy spin-excitation), it is necessary to set cdft_guru=T.

The CONSTRAINED_DFT Block is incompatible with the HUBBARD Block. To perform a constrained-DFT+U simulation with Hubbard (Uh) correction applied to the subspace in

addition to the constraining potentials (Uq/s) it is necessary to set cdft_hubbard=T. For cdft_hubbard=F (which is the default), the Hubbard correction will NOT be applied to the subspace.

Example:

```
%BLOCK CONSTRAINED_DFT
#  L  Z   Uh   Uq(UP) Uq(DOWN)  Us  N(UP) N1(DOWN) [N1(UP)-N1(DOWN)]
N1 1 -5.  0.0   11.0   11.0     0.0  2.3   1.3         0.
N2 1 -5.  0.0  -26.0  -26.0     0.0  2.7   2.7         0.
%ENDBLOCK CONSTRAINED_DFT
```

MAXIT_CDFT_U_CG

Syntax: MAXIT_CDFT_U_CG [Integer]

Description: Specifies the maximum number of iterations for the constraining potentials (Uq/s) conjugate gradients optimisation.

Default: 60

Example: MAXIT_CDFT_U_CG 5