**FALDI Advanced Options**

**FALDI TYPE [X]**

Default option **A**

Available options: A, B, C, D

*Controls the base algorithm used by FALDI, ranging from* ***A*** *to* ***D*** *(and as detailed by Cooper et al 2022)*.

*Syntax*:

FALDI TYPE D

**Isopycnic Transformations**

Default option: On

Available Options: ON, OFF, FINAL

*Controls whether or not to perform Isopycnic Transformations on the various FALDI fields. ‘ON’ will apply isopycnic transformations on all FALDI fields throughout the Orthodox, LO and LDO processes. ‘FINAL’ will only apply isopycnic transformations on the final produced density matrices*

*Syntax:*

ISOPYCNIC OFF

**Selection of overlap algorithm**

Default option: Orthodox

Available options: NONE, ORTHODOX, LO, LDO

*Controls the overlap algorithm used during calculation of density matrices. ‘Orthodox’ will calculate the QTAIM delocalization and localization indices, ‘None’ will calculate the QTAIM delocalization indices but without performing diagonalization of the matrices, ‘LO’ uses the Localized-Overlap algorithm and ‘LDO’ uses the Localized-Delocalized-Overlap algorithm*

*Syntax*:

OVERLAP LDO

**NDF Cutoff numbers**

Default option: 1 x 10–7

Available options: LNDF, DNDF

*Controls the minimum eigenvalue of NDFs saved, and printed, in all FALDI calculations. All NDFs with eigenvalues lower than the cutoff will be discarded after initial diagonalization. ‘LNDF’ controls localized NDF’s cutoffs, and ‘DNDF’ controls delocalized NDF’s cutoffs.*

*Syntax:*

CUTOFF LNDF 0.00000001

CUTOFF DNDF 1E-08

**Printing Atomic Overlap Matrices**

Default option: off

*If present, all atomic overlap matrices will be saved to a text file*

*Syntax:*

PRINT AOM