

U S E R ' S G U I D E

T D A P 2.0

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<http://everest.iphy.ac.cn/tdap>

Contents

1	INTRODUCTION	2
2	Analysis	3
2.1	Tuned electric field	3
2.1.1	Time-dependent electric field	4
2.1.2	Space nonuniform electric field	4
2.1.3	Restart a TDDFT-MD calculation	4

1 INTRODUCTION

The time-dependent DFT calculation package, named as ‘TDAP’, is aimed at carrying a non-adiabatic calculation with the full solution of time-dependent Schrodinger equation. Be aware that since the time-dependent Schrodinger equation is a one-order partial differential equation, it is a initial value problem instead of a boundary value problem. Thus, the solution method is to solve a time-evolving equation $\psi(t + dt) = \psi(t) \exp(-idtH)$ instead of a diagonalize H with $H\psi = E\psi$.

SolutionMethod (*String*): Character string to chose between diagonalization (**diagon**) or Order-N (**OrderN**) solution of the LDA Hamiltonian or the TDDFT solver (**evolve**).

Note: Always use evolve to do the TDDFT calculation, otherwise all the parameters listed below will not be read.

Default value: **diagon**

TD.FinalTimeStep (*Integer*): Final time step of the TD simulation.

Note: The number of BOMD steps is $\max(\text{MD.FinalTimeStep} - \text{TD.FinalTimeStep}, 1)$

Default value: **1**

TD.LengthTimeStep (*Real Time*): Length of the time step of the TD simulation.

Note: Best to be the same as MD.LengthTimeStep. Unit in fs.

Default value: **1.0 fs**

TD.EmptyBands (*Integer*): The number of unoccupied bands to be considered in density matrix calculation, etc.

Default value: **5**

TD.PopulationTransition (*data block*): Includes arbitrary number of lines. Each line with the format :

Start Band – End band – Jumped Electrons

Start Band is The band from which the electron is excited. If ≥ 0 , no excitation occurs.

End band is The band to which the electron is excited. Jumped Electrons is the number of electrons pumped from Start Band to End band.

For instance:

```
%block TD.PopulationTransition
-1 2 0.5
-1 1 0.5
%endblock TD.PopulationTransition
```

Means that 0.5 electrons are pumped each from the HOMO band to the LUMO band and the band higher than LUMO.

Default value: **No default values**

2 Analysis

TD.WriteDMOfSelectiveOrbitals (*logical*): Whether to output the partial DM of certain band and orbital projection.

Default value: false

TD.PartialDMBand (*data block*): Specify the band to output and orbital projection. See also **TD.PartialDMSumOrbitals**.

Multiple lines with each of them include one band index. The corresponding charge density will be projected to the selected orbital blocks, and output to file: *chgBand Index.txt*

For instance:

```
%block PartialDMBand
1
2
%endblock PartialDMBand
```

will analysis the band 1-2 and projected them to the orbital blocks. *Default value: No default values*

TD.PartialDMSumOrbitals (*data block*): Specify orbital blocks for projection. See also **TD.PartialDMBand**.

Multiple lines with each of them include the start index and the end index of the orbital. The corresponding charge density will be projected to the selected orbital blocks, and output to file: *chgBand Index.txt*

For instance:

```
%block PartialDMSumOrbitals
1 10
11 22
%endblock PartialDMSumOrbitals
```

will analysis the selected band (using **TD.PartialDMBand**) and projected them to the two orbital blocks: 1 to 10 and 11 to 22. *Default value: No default values*

2.1 Tuned electric field

The electric field can be tuned to change across z direction of the cell or change with time. Basic concept and cautions in adding electric field please refer to the **ExternalElectricField** tag, which control the value of \mathbf{E}_0 .

2.1.1 Time-dependent electric field

For the time-dependent changes, a Gaussian form wavepackage is implemented as:

$$\mathbf{E}(t) = \mathbf{E}_0 \cos(2\pi ft) \exp\left(-\frac{(t - t_0)^2}{2\sigma^2}\right)$$

TD.LightFrequency (*Real*): The frequency f of the electric field.

Default value: 0.5 fs

TD.LightInitialTime (*Real time*): The initial time t_0 to introduce the electric field.

Default value: 100.0 fs

TD.LightTimeScale (*Real time*): The peak width σ of the wavepackage.

Default value: 25.0 fs

2.1.2 Space nonuniform electric field

For the space-domain changes, only a function with selecting slab (z_{max} to z_{min}) is implemented as:

$$\mathbf{E}(t, z) = \mathbf{E}(t)\theta(z - z_{min})\theta(z_{max} - z)$$

TD.EfZmin (*Real*): The lower boundary of the electric field. Unit in percent of the cell vector.

Default value: 0.333

TD.EfZmax (*Real*): The upper boundary of the electric field. Unit in percent of the cell vector.

Default value: 0.666

2.1.3 Restart a TDDFT-MD calculation

To restart a calculation, or to analyse the charge density at certain step, the wavefunction and the atomic positions are needed. The atomic positions can be obtained by select certain lines in the file systemLabel.MD_CAR, and the wavefunction should be output using the following tag:

TD.WriteWaveFunctionStep (*integer*): If TD.WriteWaveFunctionStep = x, it means to output the wavefunction every x step to the file systemLabel.step.TDWFSX. *step* is the certain step at which the wavefunction is output.

Default value: 1000

TD.ReadWaveFunction (*logical*): Whether to read wavefunction from the file systemLabel.TDWFSX. Note: the systemLabel is not followed by *step*.

Default value: false