MultiSpec reference guide

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Contents

1 Exciton module

Exciton module is the main module that computes spectra. Currently only linear IR and Raman spectra are implemented.

1.1 Input parameters

-- **dt**: (`double`) time step between frames in ps.

-- **tc**: (`double`) correlation time for 1D time-correlation functions.

-- **H**: (`string`) name of the file containing Hamiltonian trajectory.

-- **D**: (`string`) name of the file containing transition dipole trajectory.

-- **P**: (`string`) name of the file containing transition polarizability trajectory.

-- **IR**: (`bool`) calculate linear IR spectra, options: {1,0}.

-- **Raman**: (`bool`) calculate Raman spectra, options: {1,0}. This will calculate VV, VH, isotropic, and unpolarized Raman spectra.

-- **nframes**: (`int`) how many frames are stored in trajectory files.

-- **nchrom**: (`int`) total number of chromophores.

-- **T1**: (`double`) T_1 time, life-time of the first exited state.

-- **navg**: (`int`) the number of segments the input trajectories will be divided into and used for statistical averaging.

-- **tsep**: (`double`) time separation in ps between segments.

-- **w_avg**: (`double`) average frequency (optional) helps mitigate numerical instabilities.

2 Water module

Water module generates an input for the exciton module. The input consists of excitonic hamiltonian trajectory as well as transition dipole and transition polarizability trajectories for IR, Raman, and SFG calculations.

2.1 Input parameters

-- **xtc**: (`string`) path to gromacs *.xtc file.

-- **gro_file**: (`string`) path to gromacs *.gro file.

-- **IR**: (`bool`) calculate transition dipole derivative moments for IR spectra, options: {1,0}.

-- **Raman**: (`bool`) calculate transition polarizability trajectories for Raman spectra, options: {1,0}.

-- **SFG**: (`bool`) calculate transition polarizability and transition dipole trajectories for SFG spectra, options: {1,0}.

-- **nframes**: (`int`) how many frames read from *.xtc file and process.

-- **charge_file**: (`string`) path to charge file. Charge file is a simple two-column file containing atom names matching atoms in *.gro file and corresponding charges.

-- **water_model**: (`string`) water model. Supported water models: `TIP4P`.

-- **stretch_map**: (`string`) spectroscopic map for OH and OD stretch. The following maps have been implemented so far:

  - `li_2010_tip4p` from F. Li and J. L. Skinner, J. Chem. Phys. 132, 244504 (2010)
  - `gruenbaum_tip4p_2013` from S. M. Gruenbaum et al., J. Chem. Theory Comput. 9, 3109 (2013)

-- **bend_map**: (`string`) spectroscopic map for HOH and DOD bend. The following maps have been implemented so far:

  - `ni_2015_tip4p` from Y. Ni and J. L. Skinner, J. Chem. Phys. 143, 014502 (2015)

– `ni_2015_kananenka_2019_tip4p` from Y. Ni and J. L. Skinner , J. Chem. Phys. 143, 014502 (2015) updated with HOD and D_2O bending frequencies used in Kananenka *et al.*, J. Phys. Chem. B 123, 5139-5146 (2019).

-- **spec_type**: (`string`) type of calculation that will be performed. Supported types: i) OH stretch, keyword: `wsOH`, ii) OD stretch, keyword: `wsOD`, iii) hydroxyl stretch in water isotope mixtures, keyword: `wsiso`; iv) OH-stretch fundamental-HOH bend overtone, keyword: `wswbH2O`.

-- **D2O**: (`int`) the number of D_2O molecules mixed with H_2O. This is only required for `--spec_type=wsiso`.

-- **Fc**: (`float`) OH-stretch fundamental-HOH bend overtone Fermi coupling. This is only required for `--spec_type=wswbH2O` and `--spec_type=wswbiso`.

2.2 Spectroscopic maps

3 Examples

– Generate input files for FTIR calculation of pure H_2O:

```
{PATH_TO_WATER}/water/water_gen --xtc traj.xtc --gro_file confout.gro
--charge_file q.inp --stretch_map gruenbaum_tip4p_2013 --IR
1 --Raman 0 --nframes 10 --chrom_type ws --spec_type wsOH --water_model
tip4p
```