MultiSpec reference guide

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1 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.

1.1 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:

  - F. Li and J. L. Skinner, J. Chem. Phys. 132, 244504 (2010), keyword: `skinner_tip4p_2010`
  - S. M. Gruenbaum et al., J. Chem. Theory Comput. 9, 3109 (2013), keyword: `skinner_tip4p_2010`

-- **chrom_type**: (`string`) type of chromophore for which trajectories will be generated. Supported types: i) OH(OD) stretch, keyword: `ws`.

-- **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`.

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

1.2 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