# Purpose

Derive a first-principles, SAPT-based force field.

# Relevant Literature

- VanVleet2016: 10.1021/acs.jctc.6b00209
- VanVleet2017: TBA
- McDaniel2013: 10.1021/jp3108182
- Schmidt2015: 10.1021/ar500272n
- Yu2011: 10.1021/jp204563n

# Overview

To generate a SAPT-based force field, the following inputs are required: 1. Benchmark dimer energies from SAPT, computed for a variety of dimer configurations 2. Long-range multipole moments, induced dipoles, and dispersion parameters, computed from monomer properties (and BS-ISA in particular) 3. Short-range exponents computed from monomer properties (and BS-ISA in particular) 4. Short-range pre-factors fit to dimer energies

The following scripts are designed to simplify (as much as is possible) the workflow for force field generation.

# Method

1. Generate the necessary input files upon which the scripts in step #2 depend. The following files must be manually created/edited, and can all be found in the templates subdirectory (with an example set of input files given for the pyridine dimer):
    1. dimer_info.dat
        - For each monomer, list the monomer's name and the charge on the
        - monomer. The appropriate file format should be clear from the pyridine example.
        - In the manner described in dimer_info.dat, list all midbonds that should be added between monomers. Midbonds are important for running accurate SAPT calcuations; see Yu2011 for details.
    2. generate_grid_settings.inp
        - This is the input file for GenerateGridPoints, which generates the dimer configurations for running SAPT calculations. The input file is commented so as to be self-explanatory; you will need to change (at the very least) the 1st, 3rd, and 4th input sections based on the identities of the two monomers
    3. MONA_MONB.inp (where MONA and MONB are replaced by the monomer names listed in dimer_info.dat)
        - This file contains a title line (line 1), and (for each monomer) the number of atoms followed by a list of coordinates in .xyz format. See pyridine_pyridine.inp for an example.

4. MONA.atomtypes, MONB.atomtypes
    - Each .atomtypes file has the format of a .xyz file, where the element names have been replaced by atomtypes. This file will be used to generate the CamCASP input files needed for ISA calculations, and is also necessary for pre-processing the input files for force field fitting.

2. To generate all files necessary to run force field calculations, run the following pre-processing scripts (from this main directory).

```
./scripts/make_geometries.sh

./scripts/get_global_coordinates.py

./scripts/submit_ip_calcs.py
```

(wait until IP calculation is finished)

```
./scripts/make_sapt_ifiles.py

./scripts/make_isa_files.py

./scripts/make_dispersion_files.py
```

3. Submit all SAPT and ISA calculations to relevant locations. At the time of this writing, SAPT calculations should preferably be run on HCTC (Condor). ISA and dispersion calculations should be run on Phoenix using Camcasp 5.8. Copy all output files back to Pople.

4. Workup the results of the SAPT and ISA calculations by running the following post-processing scripts:

```
./scripts/workup_sapt_energies.py

./scripts/workup_dispersion_files.sh
```

(Depending on the force field, dynamic polarizabilities may need to be added to templates/dispersion_base_constraints.index before running this script. See Jesse McDaniel's thesis and \cite{McDaniel2013} for a full description of the paramterization process for dispersion coefficients.)

```
./scripts/workup_drude_files.sh
```

(Depending on the force field, static polarizabilities may need to be added to templates/drude_base_constraints.index before running this script. See Jesse McDaniel's thesis and \cite{McDaniel2013} for a full description of the paramterization process for drude oscillator charges.)

```
./scripts/workup_isa_charges.py

./scripts/workup_isa_exponents.py
```

After running these scripts, you should have the SAPT energies, long-range coefficients, and short-range exponents required to run the force fitting code (which is needed to generate short-range pre-factors, see \cite{VanVleet2016}). The proper running of this code is described in the POInter documentation, see

https://git.chem.wisc.edu/schmidt/force_fields/wikis/home

# Overview of Important Files

- dimer_info.dat <- monomer names and midbond positions
- dispersion_template.clt <- CamCASP input file for getting induction and
- dispersion paramters
- generate_grid_settings.inp <- geometry configuration settings
- isa_template.clt <- CamCASP input file for getting ISA exponents
- pbe0_template.com <- DF-DFT-SAPT template for the PBE0 functional
- pyridine.atomtypes <- change elements to atomtypes; only matters for
- dispersion
- pyridine_pyridine.inp <- monomer geometries

For most systems, only dimer_info.dat, the .inp files, and the .atomtypes file will need to be changed. The examples provided for these files should hopefully make the format self-explanatory.

# System Requirements

Python dependencies: * numpy * scipy * chemistry (mvanvleet package; not standard, so this needs to be * downloaded and added to your `$PYTHONPATH`)