raman-sc / **VASP**

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1 contributor

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vasp_raman.py

Raman off-resonant activity calculator using VASP as a back-end.

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Theory

In order to calculate off-resonance Raman activity of a mode, one needs to compute the derivative of the polarizability (or macroscopic dielectric tensor) with respect to that normal mode coordinate: `dP/dQ` (or `de/dQ`).
Thus, two ingredients are required:

1. Phonons at Γ-point
2. Macroscopic dielectric tensor

Phonons at Γ-point

In VASP, phonons at Γ-point can be computed using either:

- finite displacements: `IBRION=5` or `IBRION=6`; or
- density functional perturbation theory (DFPT): `IBRION=7` or `IBRION=8`.

Only finite displacements are available when hybrid functional is employed.

Macroscopic dielectric tensor

In VASP, macroscopic dielectric tensor can be computed using either:

- DFPT: `LEPSILON=.TRUE.`
- or from frequency dependent dielectric matrix calculation: `LOPTICS=.TRUE.`.

In the latter case, hybrids functionals could be employed.
For a more formal description of the method see D. Porezag, M.R. Pederson, PRB, 54, 7830 (1996).

Installation

Python >= 2.6 is required. Just copy `vasp_raman.py` in the `$PATH` and run! No external dependencies.

Global variables

`vasp_raman.py` **requires** two environmental variables to be set:

- `VASP_RAMAN_PARAMS` is defined as `FIRST-MODE_LAST-MODE_NDERIV_STEPSIZE` where:
  - `FIRST_MODE` - integer, first mode for which derivative of the polarizability is computed
  - `LAST-MODE` - integer, last mode for which derivative of the polarizability is computed
  - `NDERIV` - integer, scheme for finite difference, **currently** only value `2` is supported
  - `STEPSIZE` - float, step-size for finite difference, in Angstroms

  Example: `VASP_RAMAN_PARAMS=01_10_2_0.01`
- `VASP_RAMAN_RUN` the command to execute VASP (can contain MPI call):
  Example: `VASP_RAMAN_RUN='aprun -B /u/afonari/vasp.5.3.2/vasp.5.3/vasp &> job.out'`

Both variables should be `exported` (in Bash language) before running `vasp_raman.py`.

An example of PBS script:

```
#!/bin/bash
#PBS -l select=1:ncpus=32:mpiprocs=32
#PBS -l walltime=01:00:00
#PBS -q debug
#PBS -j oe
#PBS -N Example
#PBS -V

cd $PBS_O_WORKDIR

ulimit -s unlimited  # remove limit on stack size

export VASP_RAMAN_RUN='aprun -B /u/afonari/vasp.5.3.2/vasp.5.3/vasp &> job.out'
export VASP_RAMAN_PARAMS='01_10_2_0.01'

python27 vasp_raman.py > vasp_raman.out
```

An example of bash script (in case no scheduler is installed):

```
#!/bin/bash

# suggested by Ricardo Faccio, Universidad de la República, Montevideo, Uruguay

# OpenMP variables
#export OMP_NUM_THREADS=1
#export MKL_NUM_THREADS=1

# vasp_raman.py variables
export VASP_RAMAN_RUN='mpirun -np 4 vasp5.3.5_par'
export VASP_RAMAN_PARAMS='01_06_2_0.01'

python /home/user/bin/vasp_raman.py > vasp_raman.out
```

Examples

- Raman activity spectrum for Si using VASP
- Raman activity spectrum for Si using VTST tools

- Raman activity spectrum for cyclopentadiene using VASP
- Raman activity spectrum for Si using VTST tools and PW91 functional

Changelog

0.6 (will be released soon)

- ADDED: ability to use phonons obtained from the vtst tools
- FIX: cleaned `POSCAR` parsing code

0.5.1

- FIX: contributors and version are now in the output
- FIX: Cyclopentadiene example is now fully consistent with the version

0.5

- Basic working functionality

How to cite

Use Bibtext or RIS file for citation.

Contributors

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