Phonon Analysis using Real-Space Multigrid Method and VISION

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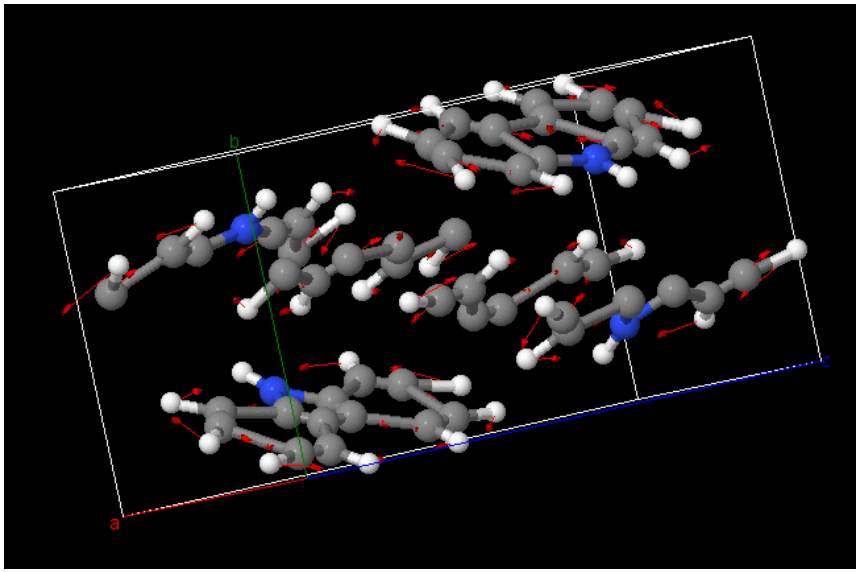
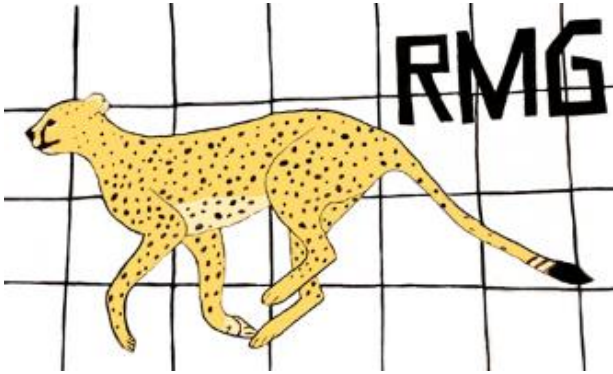
OUTLINE

- Real-Space Multigrid code: RMG
- VISION Spectrometer
- Calculations on various systems:
  - Zirconium(II) Hydride
  - ZIF-8

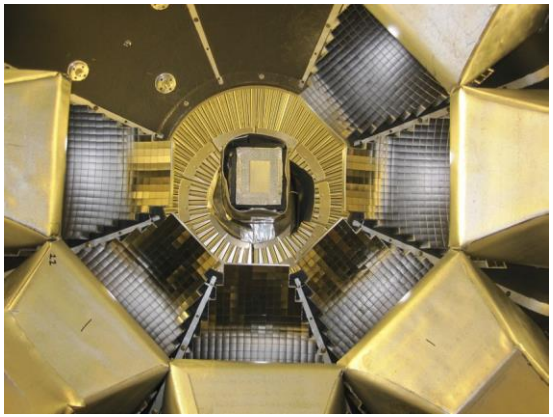


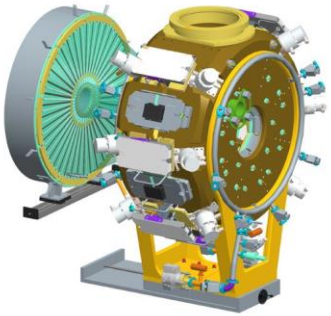
RMG code

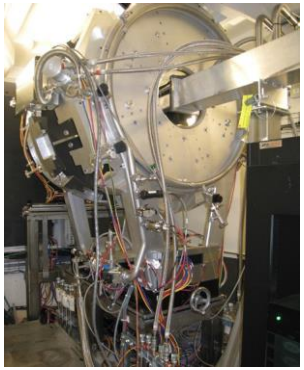


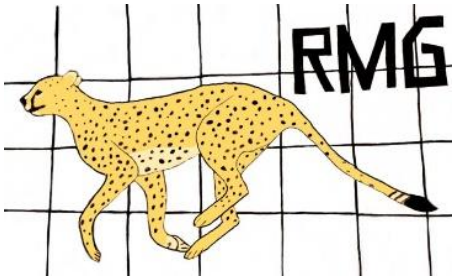
- **RMG** (**R**eal-space **M**ulti**G**rid) is an open source electronic structure code for DFT calculations (http://www.rmgdft.org)
- It uses real space grids to represent wave functions, charge densities and ionic potentials.
- Highlighted features:
  - Real space based
  - Multi-architecture support: Unix/Linux, Windows and Mac OS
  - GPU accelerated
  - Parallelizes to 200k cores and 10k GPUs: Titan, Blue Waters, Summit
- Suitable for phonon calculations, which may need to handle hundreds to thousands of atoms in enlarged supercells

High-throughput vibrational analysis of neutron scattering data









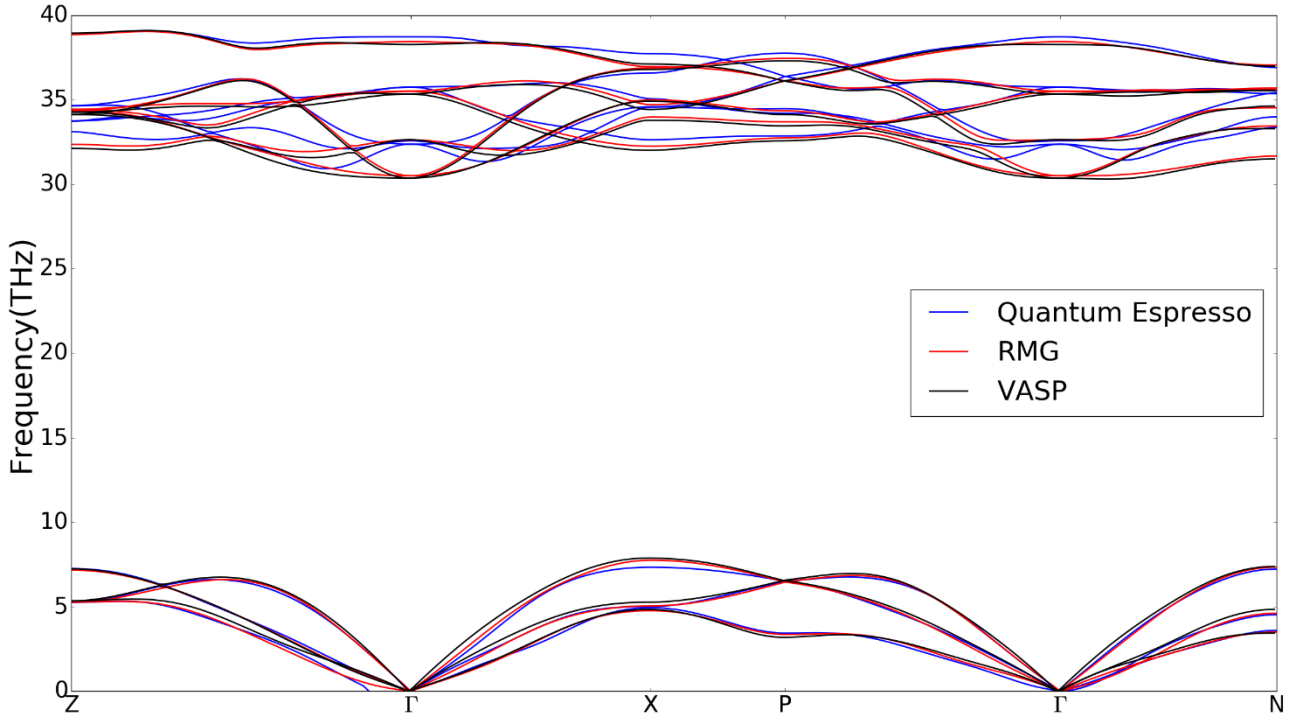
"Vision" instrument at the Spallation Neutron Source (SNS)

- Highest resolution broadband inelastic neutron scattering (INS) spectrometer in the world.
- World's first high throughput INS instrument.
- Vibrational spectra in "real-time."

RMG code

- Is being incorporated into neutron spectroscopy analysis software.
- Will enable high throughput collection and vibrational analysis of neutron scattering data.

Calculation: Zirconium (II) Hydride (ZrH_2)

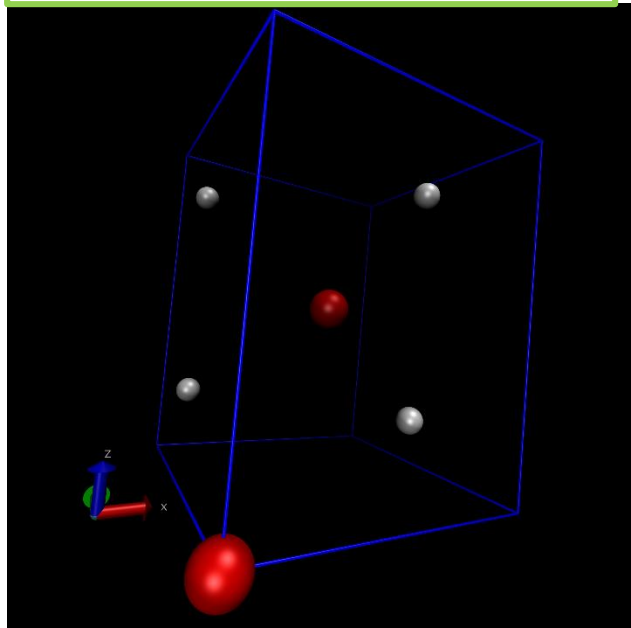


Phonon band structure calculated by RMG, VASP and Quantum Espresso

- Typical system
- Metallic
- Anharmonicity

Computational Details

- Chemical formula: ZrH_2 (6 atoms per unit cell)
- Space group: I4/mmm
- Size: 3.520*3.520*4.449 $Å^3$
- Supercell: [5 5 3], 450 atoms



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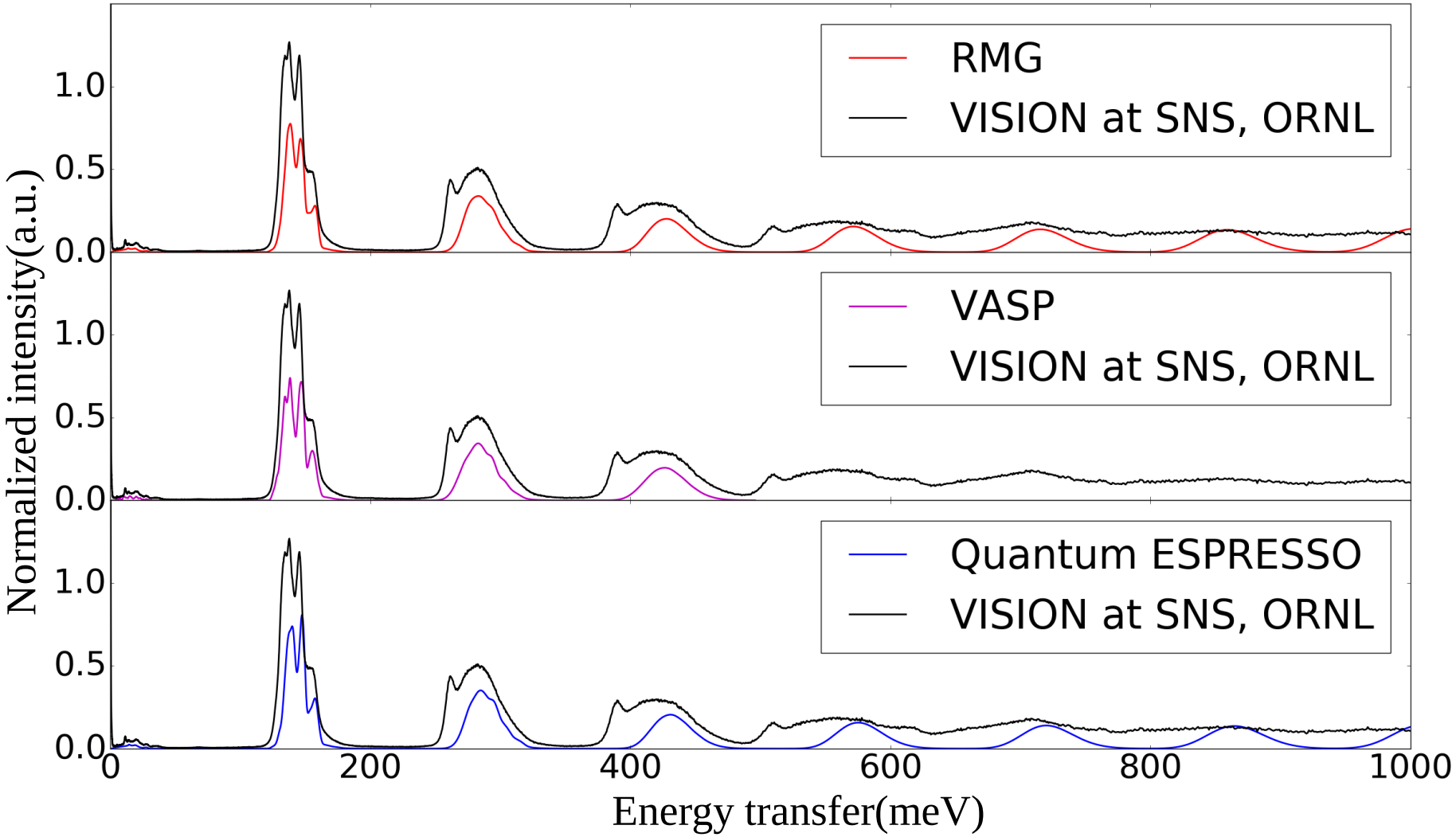
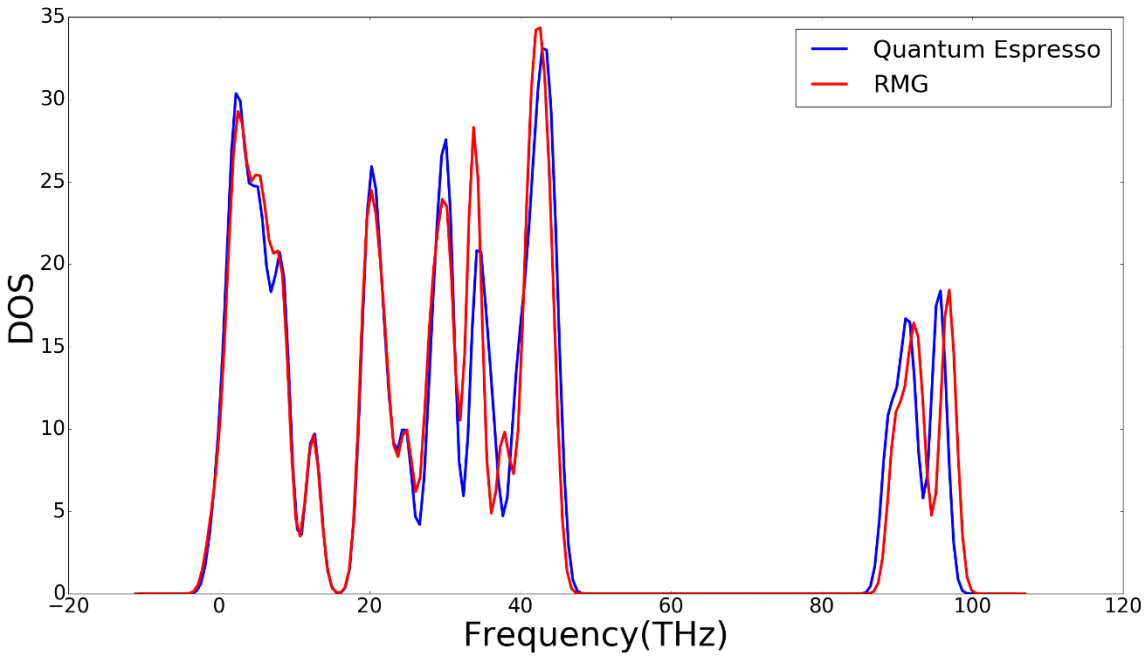


Intensity comparison among RMG, VASP, Quantum Espresso and Experimental data

Calculation: ZIF-8 ($C_{96}H_{120}N_{48}Zn_{12}$)



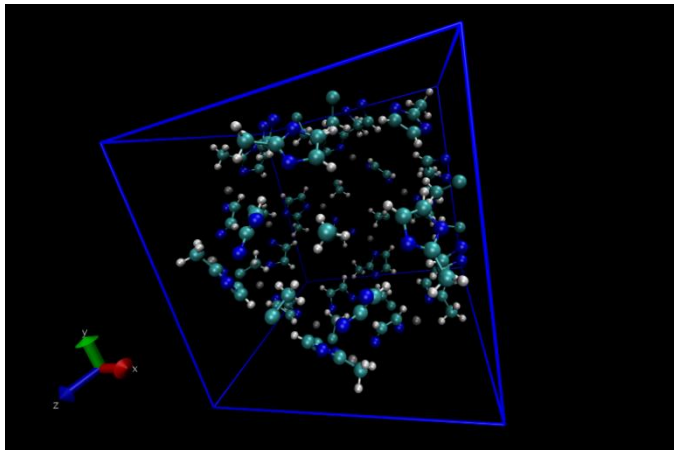
Phonon DOS comparison between RMG and Quantum Espresso

- ○ Small discrepancy at around 38 THz
- ✓ Very good agreement with each other

❖ Large system

Computational Details

- Chemical formula: $C_{96}H_{120}N_{48}Zn_{12}$ (276 atoms per unit cell)
- Space group: $I\bar{4}3m$
- Supercell: [1 1 1]



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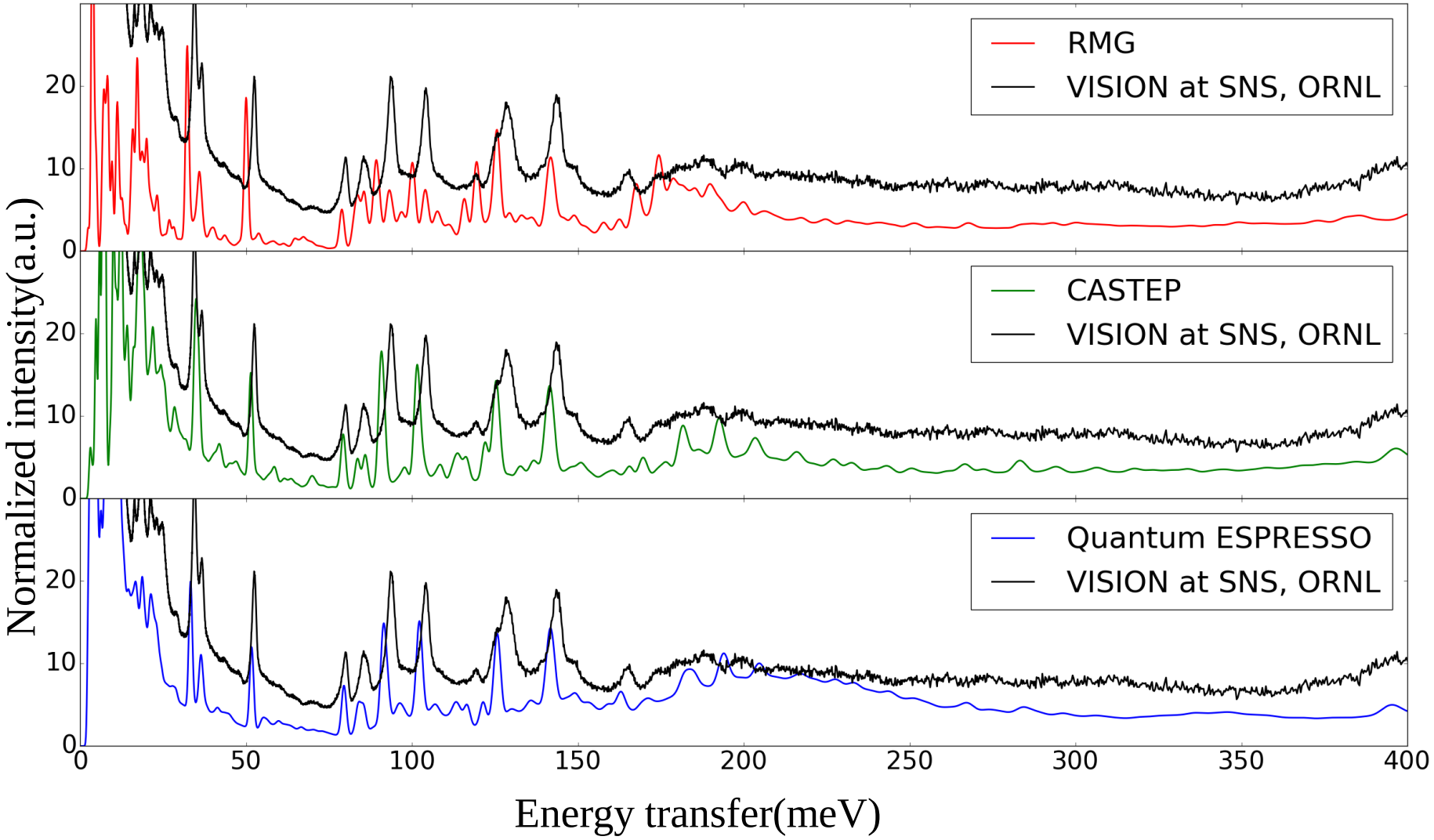

Intensity comparison among RMG, CASTEP, Quantum Espresso and Experimental data

Thank you!