We describe method developments and their implementation in the WEST code; WEST is a massively parallel code for large-scale many-body perturbation theory calculations (GW and BSE) with scalar and fully relativistic pseudopotentials.

Large-scale many-body perturbation theory

**Distinctive features**
- Low-rank decomposition of dielectric matrices (no explicit diagonalization and storage of the full matrix)
- No explicit calculation of virtual electronic states
- GW with full frequency integration
- GW starting from semi-local and hybrid DFT
- Parallelization demonstrated over 500k cores on ANL Mira and 200k cores on ANL Theta

**New Features**
- Electron-phonon self-energy evaluated without computing virtual electronic states
- GW calculations with spin-orbit coupling
- New hybrid functionals derived from GW
- WEST-Qbox coupling for BSE and GW
- Restructured I/O in JSON format, enabling seamless integration with WESTpy and compatibility with Jupyter notebooks

**Software development**
- A dedicated GitLab server is operational
- Public releases are mirrored on Github
- Continuous Integration is used to verify the integrity of the code at every step of the development
- Documentation is automatically generated using Sphinx
- License under the open-source GPLv3

**WESTpy and REST API tutorials**
- WESTpy is a python package designed to assist users of the WEST code in pre- and post-processing operations
- REST API tutorials allow users to run the codes as-a-service, without learning how to install

http://www.west-code.org/doc/westpy/latest/

**Electron-phonon coupling**
- Efficient evaluation of e-h self-energies using GW quasi-particle energies
- No virtual electronic states
- Lanczos algorithm is utilized to compute all self-energies over the full frequency spectrum
- Temperature dependent computational spectroscopy
- Lifetimes to be used in Boltzmann Transport Equation (BTE)
- Combined Approach

**Electron-electron and electron-phonon lifetimes**
- Computation of electron-electron and electron-phonon self-energies are combined
- Lifetimes can be efficiently computed in nanoparticles with more than several hundred electrons and phonon modes

**Verification**
- G\_W\_e for solids: comparison between results obtained with West and those reported by D. Nalos et al, PRB 2018 (G\_W\_e & SLDA with the exciting code).
- Systematic improvement of DFT results is ~2x worse than in DFT (DFT(PBE))
- Ongoing work: impact of semi-core states in G\_W\_e calculations
- Two PP for WO\_3, PPR (28 VE for W), PP2 (14 VE for W) yield the same results at the DFT level but different results for CSM and band gap at the G\_W\_e level of theory

**Liquids and solid/liquid interfaces**
- Dielectric properties of interfaces expressed in terms of those of sub-systems
- Design of local hybrid functional for modeling heterogeneous systems

**Hybrid functional for interfaces**
- Dielectric constant evaluated using a finite field method (with Qbox)
- Local hybrid functional
- Dielectric constant constant evaluated using a finite field method (with Qbox)
- Suggested hybrid functional
- We revisited the experimental literature on the EA of water.
- We computed the electron affinity (EA) of bulk water and its surface.
- Suggested hybrid functional

**WEST porting to new platforms**
- WEST was ported to Intel Xeon Phi KNL platforms:
  - Theta at ALCF
  - Cori at NERSC
- Code optimization & parallelization paves the way to an efficient utilization of the Aurora platform at ALCF

**Ongoing and future work**
- Investigate the accuracy of pseudopotentials for MBPT calculations
- Develop and implement new algorithms to investigate ultrafast time-resolved processes
- Enable on-the-fly calculations of spectroscopic properties

**Table 4: Energy gap of Si-NCs.**

<table>
<thead>
<tr>
<th>Compound</th>
<th>Energy Gap (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si-NC</td>
<td>1.73 (2.00)</td>
</tr>
<tr>
<td>Si</td>
<td>1.53 (1.80)</td>
</tr>
<tr>
<td>Si-NC</td>
<td>1.69 (1.96)</td>
</tr>
</tbody>
</table>

**Figure 1: Electronic lifetimes.**