

Release notes for RESCU-2.3.0

1. **Improved** function `dfpt - raman` yields the 2nd order non-linear optical susceptibility, includes LO-phonon corrections to the Raman tensor. It also computes the Raman intensities and spectra for polarized and polarization-averaged experimental setups. The new functionalities are supported with various visualization tools.
2. **New** `berry-curvature` calculation type allows computing the Berry curvature of two-dimensional materials.
3. **New** `stm-current` calculation type allows computing sample-tip current using Bardeen's theory.
4. **New** `dfpt` solver PCFSI based Chebyshev filtering activated by setting `dfpt.method = 'cfsi'`. It is generally faster and has significantly lower memory footprint compared with the state-of-the-art CG solver when solving large systems on parallel computing platforms.
5. **New** restart feature and keyword `option.timeLimit` allow seamlessly restarting a `self-consistent` calculation that runs out of time on a cluster.
6. **New** keyword `option.precision` allows to simply choose between real space or planewaves, and low, medium or high accuracy; with the values: 'real-low', 'real-med', 'real-high', 'pw-low', 'pw-med', 'pw-high'.
7. **New** feature allows changing the value of certain keywords at run time using the file `rescu_runtime.input`.
8. **New** projected local DOS (PLDOS) capability of the LDOS calculator. The PLDOS basis is specified in the same way as the projected DOS (PDOS).
9. **New** output format. In addition to the standard MAT-files, RESCU also writes the following results in formats compatible with third-party analysis tools:
 - a) `band-structure`: `BandStructure.txt`, `PartialWeightsBandStructure.txt` (if band decomposition is activated)
 - b) `band-unfolding`: `UnfoldedBandStructure.txt`
 - c) `dos`: `DensityOfStates.txt`
 - d) `dfpt-phonon-bs`, `dfpt-phonon-dos`: phonon modes written to `PhononBandStructure.yaml`.
 - e) `density`: `Density.txt` (modified POSCAR)
 - f) `ldos`: `LocalDensityOfStates.txt` (modified POSCAR)
 - g) `potential`: `Potential.txt` (modified POSCAR)
 - h) `wavefunction`: `Wavefunction.txt` (modified POSCAR)

Note: Unless otherwise specified, bug fixes do not influence previous results.