

Release notes for RESCU-2.1.0

1. **New** Density function perturbation theory solver. The solver can compute the following properties of gapped materials: polarizability, dielectric tensor, dynamical matrix, Born effective charges, phonon band-structure and density of states, infrared spectrum, reflectance, transmittance. DFPT is implemented in the real space grid framework only. The LDA and GGA may be used together with norm-conserving pseudopotentials. The code is parallelized over bands, k-point and spin and may exploit GPU devices.
2. **New** real space DFT+U solver. The Hubbard interaction may be included in real space calculations.
3. **New** GPU LCAO solver. Atomic orbital calculations may now exploit GPU devices.
4. **New** PEXSI LCAO solver. The PEXSI (Pole Expansion + Selected Inversion) algorithm has been implemented. The algorithm is most powerful for large and low-dimensional systems (e.g. nanotubes). The peanut contour introduced by Lin is used for the pole expansion. A principal layer order inversion algorithm is used for the selected inversion. The code may exploit GPU devices.
5. **New** band unfolding calculation type. An effective spectral function can be calculated for a primitive cell from a supercell's wavefunctions, a procedure called band unfolding. The spectral function is stored in the output `band.specFun`. The rescu plotting routine will every band structure point using a marker size proportional to the value of the spectral function.
6. **New** output option `option.savePartialWeights`. If the value is true, every electronic state is decomposed into its atomic orbital components and the weights are stored in `HDF5/LCAO/partialWeight#`.
7. **New** output LCAO orbital info. The orbital information is saved in a clear format in `LCAO.orbInfo`. Users will find it useful to analyze Mulliken charge or band decomposition data for example.

8. **Improved** relaxation engine. The optimization algorithms have been made more robust by introducing a few restarting strategies. The eggbox effect is reduced or eliminated by using better interpolation methods.
9. **Improved** GGA potential. Certain combinations of material and simulation parameters introduce spurious variations in the GGA potential, preventing the converge of the self-consistent procedure at high accuracy. The GGA kernel undergoes a smoothing procedure resolving the issue.
10. **Improved** MBJ functional. The MBJ functional smoothly tend to the LDA in low density regions. This improves the stability for slab geometries or hollow systems like nanotubes.

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