

Release notes for RESCU-2.2.0

1. **New** function `dfpt-raman` yields the Raman tensor and intensity.
2. **New** function `wannier` computes maximally localized Wannier functions (MLWF). The function supports all spin types, entangled bands, inner energy windows, etc., but it is only available with the LCAO framework.
3. **New** implementation of HSE-like hybrid functionals: NOPAIN2. The revised NOPAIN implementation includes a high momentum correction (controlled by the keyword `Exx.highGcorr`) which allows accurate calculation with a reduced planewave cutoff, thus saving significant time and memory.
4. **New** implementation of HSE-like hybrid functionals supports all spin types.
5. **New** hybrid functionals. The following parameters are added to the hybrid function interface: `Exx.beta` (β), `Exx.omegaHF` (ω_{HF}), `Exx.omegaPBE` (ω_{PBE}).
The resulting functional is defined as
$$E_{xc} = \beta E_x^{HF,SR}(\omega_{HF}) + (1 - \beta) E_x^{PBE,SR}(\omega_{PBE}) + E_x^{PBE,LR}(\omega_{PBE}) + E_c^{PBE}$$
6. **New** Mobcal support. The mobility calculator Mobcal now has a RESCU interface.
7. **New** GPU support for hybrid functional calculations
8. **New** parallel RESCU supports all MATLAB version up to 2019a.
9. **Improved** real space solvers' efficiency. Notable, we implemented: a non-blocking planewave filter, a non-blocking Rayleigh-Ritz scheme, improved interpolation schemes.
10. **Improved** parallelization: RESCU automatically tunes parallelization parameters such as `mpi.parak`, which controls whether RESCU should parallelize over k-points and spin degrees of freedom.
11. **Improved** phonon calculations. An automatic restarting procedure is implemented.

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