

# The $\nu$ -ESPRESSO Project

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$\nu$ -ESPRESSO /'kwɒntəm-ɛ'spresəʊ/ is a collaborative, open-source project<sup>1</sup> for quantum-mechanical simulations of extended or isolated systems based on density-functional theory, periodic-boundary conditions, plane-waves, and norm-conserving or ultrasoft pseudopotentials.  $\nu$ -ESPRESSO integrates in a new, modular and multi-platform framework the electronic-structure packages developed in the last two decades by groups in Trieste<sup>2</sup> and in Lausanne,<sup>3</sup> and rewritten for this project.

The  $\nu$ -ESPRESSO core is based on the self-consistent determination of ground-state energies and forces, Car-Parrinello molecular dynamics, and linear-response theory, implemented in a fast and scalable architecture that includes extensive use of libraries (BLAS, LAPACK, MKL, FFTW), optimal parallelization over plane-waves, FFT grids, and k-point meshes, and

(CP only) a very efficient implementation of Gamma-sampling and ultrasoft box-grids. Advanced capabilities include the calculation of phonon eigenvalues and eigenvectors, effective charges and dielectric constants, Berry-phase polarization, electron-phonon coupling and phonon lifetimes, infrared and Raman cross sections, spin-orbit coupling and non-collinear magnetism, electric field gradients, nudged elastic-band methods and string dynamics, ensemble density-functional theory, maximally-localized Wannier functions, and molecular dynamics in the microcanonical, canonical, isoenthalpic, and isoelectric ensembles. Input via the graphical user interface PWgui is integrated into the package, and visualization performed via the public-domain XCrysDen package (<http://www.xcrysden.org>).

*$\nu$ -ESPRESSO stands for *Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimisation*; its development is led by the Italian National Simulation Center DEMOCRITOS (hosted by the International School of Advanced Study in Trieste), in collaboration with ICTP Trieste, CINECA Bologna, Scuola Normale Superiore in Pisa, Princeton University, MIT, and all their respective funding agencies. The package and its tutorials are distributed under the GNU General Public License and made available to the scientific community worldwide at <http://www.pwscf.org> and <http://www.democritos.it>. Electronic-structure schools and classes based on this software are periodically offered in developed and developing countries, with additional support from the UNESCO/IAEA International Center of Theoretical Physics in Trieste.*

- [1] S. Baroni, A. Dal Corso, S. de Gironcoli, P. Giannozzi, C. Cavazzoni, G. Ballabio, S. Scandolo, G. Chiarotti, P. Focher, A. Pasquarello, K. Laasonen, A. Trave, R. Car, N. Marzari, A. Kokalj, <http://www.pwscf.org/>.
- [2] *Phonons and related crystal properties from density-functional perturbation theory*, S. Baroni, S. de Gironcoli, A. Dal Corso, and P. Giannozzi, *Rev. Mod. Phys.* 73, 515-562 (2001).
- [3] *Car-Parrinello molecular dynamics with Vanderbilt ultrasoft pseudopotentials*, K. Laasonen, A. Pasquarello, R. Car, C. Lee, and D. Vanderbilt, *Phys. Rev. B* 47, 10142-10153 (1993).