

## **Workshop on Quantum Espresso**

ICHEC and the Tyndall National Institute are organising a Workshop on the theory and practical uses of Quantum ESPRESSO (QE) to take place

**at the Tyndall National Institute**

**from June 14<sup>th</sup> to June 18<sup>th</sup> 2010**

The course will be given by a world-class scientist team of QE experts and developers. Full details of the Workshop including registration details can be found here: ([http://www.ichec.ie/education\\_training/qe\\_workshop](http://www.ichec.ie/education_training/qe_workshop))

Quantum ESPRESSO is an integrated suite of computer codes for electronic structure calculations and materials modelling at the nanoscale level and has been used by some of the leading materials modelling groups worldwide in the last 20 years. It builds onto newly-restructured electronic-structure codes (PWscf, PHONON, CP90, FPMD, Wannier) that have been developed and tested by some of the original authors of novel electronic-structure algorithms - from Car-Parrinello molecular dynamics to density-functional perturbation theory. Its growing popularity is due in part to its high scalability (users regularly scale up QE codes to several hundreds of cores and sometimes a few thousand cores) as well as its flexibility in addressing a wide range of problems in materials science (for details of the codes applications see <http://www.quantum-espresso.org/whatcangedo.php>).

**QE will be of particular interest to materials modelling groups with an interest in running codes on the new PRACE petaflop systems.**

Quantum ESPRESSO is an initiative of the DEMOCRITOS National Simulation Center (Trieste), of SISSA (Trieste) and of their partners, in collaboration with CINECA National Supercomputing Center in Bologna, the Ecole Polytechnique Fédérale de Lausanne, Princeton University, the Massachusetts Institute of Technology and Oxford University.

Topics at the Workshop cover a range of contemporary QE applications, from simple electronic structure calculations, equilibrium structure and reaction paths search, to the most sophisticated theoretical spectroscopies such as nuclear magnetic resonance (NMR), electron paramagnetic resonance (EPR), optical absorption, Raman and scanning tunnel microscopy, etc.

Deadline for registration is on April 30<sup>th</sup>.

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