Atomistic *ab initio* simulations and their role in the nanoworld

Wanda Andreoni
Ecole Polytechnique Fédérale de Lausanne
Lausanne, Switzerland

During the last two decades, atomistic simulations have become an unavoidable tool for research in materials science. In particular, *ab initio* calculations are converging to the nanometer scale and can provide important new insights on a number of properties and processes that are still eluding experiment. This is the case of structural properties and chemical reactions. After introducing advanced methods currently is use for atomistic simulations, I will present a few applications, e.g., to carbon nanotubes and photovoltaics.