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2008 J. Phys.: Condens. Matter 20 064212

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J. Phys.: Condens. Matter **20** (2008) 064212 (1p) doi:10.1088/0953-8984/20/6/064212

First-principles computation of the electronic and dynamical properties of solids and nanostructures with ABINIT

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Received 17 December 2007
Published 24 January 2008
Online at stacks.iop.org/JPhysCM/20/064212

Abstract

The field of first-principles simulation of materials and nanosystems has seen an amazing development in the past twenty years. Using the density-functional theory and complementary approaches, like many-body perturbation theory, it is now possible to compute both basic quantities, like crystalline lattice parameters, and more involved properties, like optical or phonon spectra. New and improved concepts, approximations, algorithms, and numerical techniques appear every year.

In order to cope with the increasing software complexity, it became apparent over a decade ago that software engineering techniques and a group collaborative effort would be major ingredients of a successful first-principles project. The open source ABINIT project was launched in 1997; as of now, there are more than 1000 members on the main mailing list, over 40 active contributors, and more than 200 articles have been published in international journals using ABINIT.

I will present the overall structure of the package, and its main and most exciting capabilities. Specific recent examples of projects will demonstrate some of the full palette of features in ABINIT. These projects are often carried out in close collaboration with experimentalists, and ABINIT is also used by or for a number of industrial partners.

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