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The ABINIT software package : theoretical spectroscopy of materials.

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ABINIT allows one to study, from first-principles, properties of materials (also molecules, nanostructures, etc.), on the basis of Density-Functional Theory (DFT) and Many-Body Perturbation Theory. Beyond the computation of the total energy, charge density and electronic structure of such systems, ABINIT also implements many dynamical, dielectric, thermodynamical, mechanical, electronic or optical properties, at different levels of approximation. Used an estimated 1000 scientists worldwide, ABINIT is especially appreciated for its electronic, optical and vibrational spectroscopy capabilities (photoemission, optical, IR/Raman spectroscopy ...). The presentation will cover the description of ABINIT capabilities, and present some applications. ABINIT is freely available (GNU GPL) at [http://www.abinit.org]. For a recent account, see Computer Physics Communications 180 (2009) 2582–2615.