ABINIT Plugin
A versatile package for first principles periodic quantum calculations of materials and nanosystem properties

Features & Capabilities
Density-Functional Theory and Many-Body Perturbation Theory (GW Approximation) calculations. Total energy, charge density, electronic structure, many dynamical, dielectric, thermodynamical, mechanical or electronic properties at different levels of approximation.

Summary
ABINIT accurately computes many material and nano-structure properties: electronic structure, bond lengths, bond angles, primitive cell size and shape, cohesive energy, dielectric properties, vibrational properties, magnetic properties, nonlinear couplings, etc. ABINIT uses Density-Functional Theory, Density-Functional Perturbation and Many-Body Perturbation Theories together with pseudopotentials and plane-waves, Projector-Augmented Waves (PAW) or wavelets as basis functions.

ABINIT technology is well suited for problems in solids state physics, materials science, chemistry and materials engineering involving solids, molecules, surfaces and interfaces of a wide range of materials such as conductors, semiconductor and insulators.

ABINIT can be combined with TURBOMOLE, LAMMPS and MNDO within QMPOT in order to perform QM/MM or QM/QM type of simulations. This type of simulations allow to study large systems in the areas of catalysis and surface chemistry.

Finally, ABINIT can benefit from TRANSITION STATE LOCATOR in order to localize transition states using Linear / Quadratic Synchronous Transit (LST/QST) or Nudged Elastic Bands (NEB) techniques.
ABINIT in MAPS

SCIENOMICS technology is offered as a series of software plugins in the MAPS platform, which is a powerful and extendable simulation environment. Chemists, materials scientists and chemical engineers can access several molecular and thermodynamic simulation engines within MAPS in order to achieve the required quality by design. MAPS technology covers the whole range from quantum and classical simulations to mesoscopic and thermodynamic modeling.

The MAPS platform runs on several Linux and Windows® operating systems. In the area of molecular modeling MAPS includes a series of tools enabling the construction of any molecular model, finite and periodic, 3D visualization and other productivity utilities. Therefore, the ABINIT user can quickly create a periodic system, using standard sketching tools or MAPS’ crystal and surface builders, and set up calculations using the ABINIT graphical user interface which gives access to many of ABINIT advanced quantum capabilities.

Analysis tools and graphs available in MAPS enable an easy representation of ABINIT results. MAPS native client-server architecture enables best usage of available computational resources across numerous operating systems. Finally, MAPS offers efficient interaction with office productivity tools.

References

Modeling workflow with MAPS

In modern industrial R&D projects, materials scientists and engineers have to efficiently build correlations between the macroscopic properties of a system and the microscopic characteristics of the materials involved. In such a project several candidates need to be considered. Molecular simulation technologies offered within MAPS address all aspects of materials design ranging from quantum mechanics to thermodynamics and are capable of generating relevant insights for an efficient product and process design.

MAPS infrastructure offers a unique combination of simulation technology, data management via its build-in database, and Python based scripting of its functionality that enables preparation and execution of sophisticated simulation protocols. A protocol can combine all tasks a scientist needs to execute and repeat these for a large number of models.