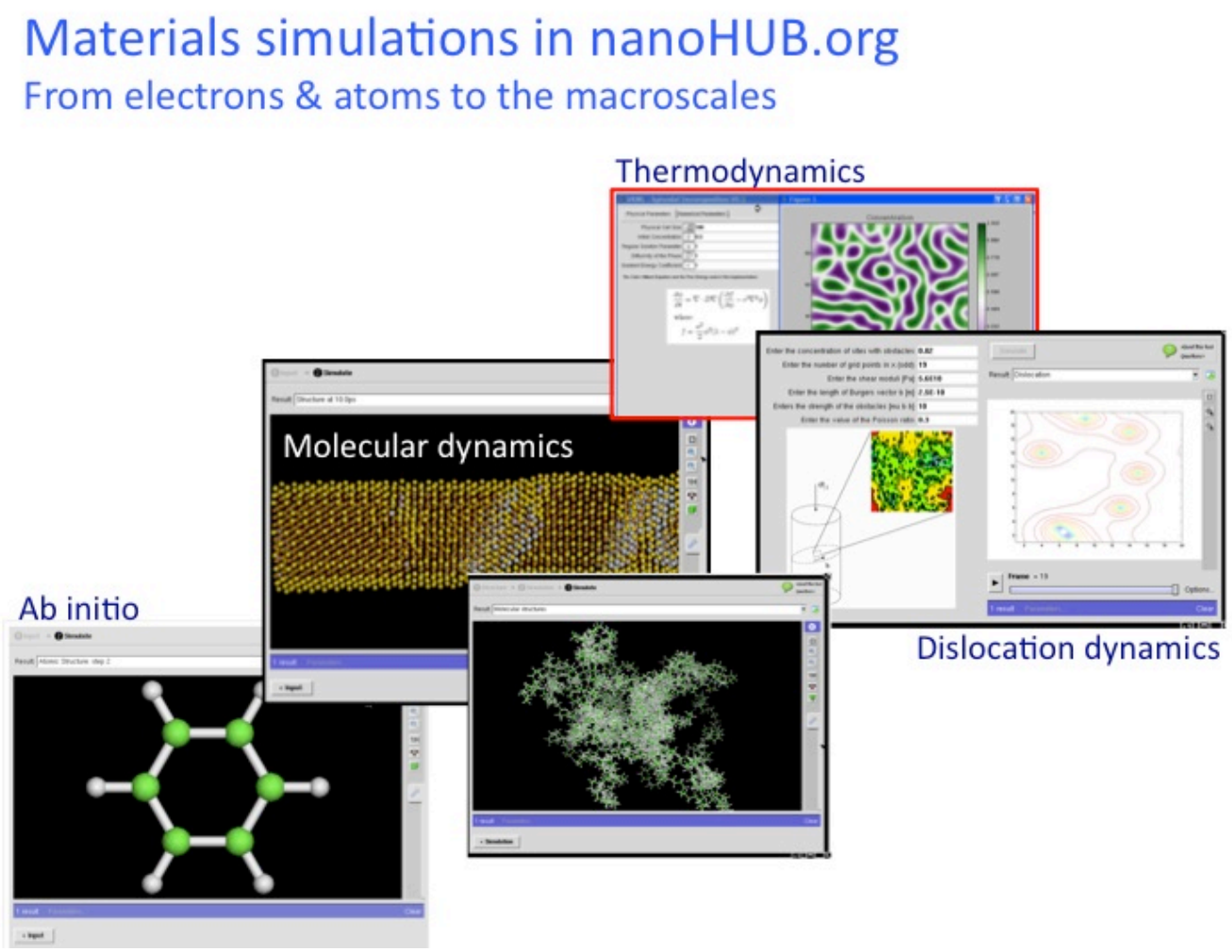
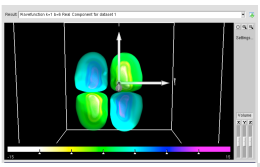
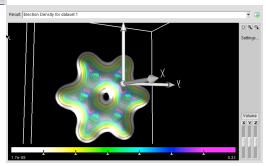
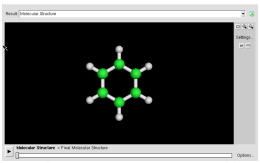
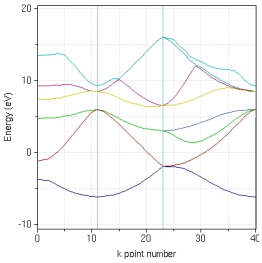
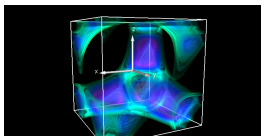
Resources for Materials Science and Engineering



Ab initio electronic structure simulation tools

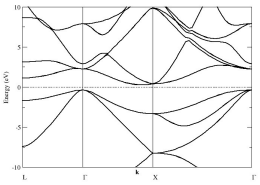
ABINIT



:ABINIT is a package whose main program allows to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory, using pseudopotentials and a planewave basis. ABINIT also includes options to optimize the geometry according to the DFT forces and stresses, or to perform molecular dynamics simulation using these forces, or to generate dynamical matrices, Born effective charges, and dielectric tensors. In addition to the main ABINIT code, different utility programs are provided.
:First Time User Guide for ABINIT on nanoHUB.org
:Official ABINIT site
:ABINIT New User Guide

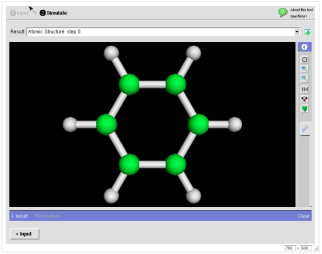
SIESTA



: Siesta is a fast electronic structure program that uses a local basis. It can produce band structures and minimum energy geometries, and can perform first principles

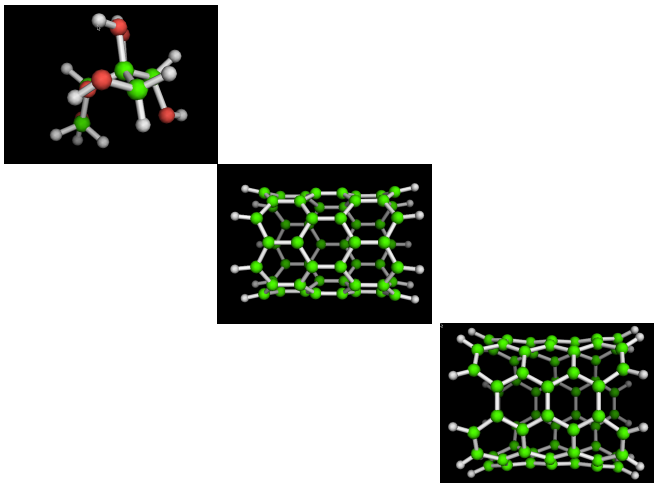
molecular dynamics calculations.
:siesta Website

nanoMATERIALS SeqQuest DFT



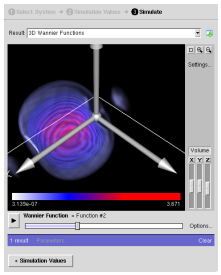
:powered by SeqQuest
:This tool provides access to the density functional theory code SeqQuest via nanoHUB.org. SeqQuest is being developed at Sandia National Laboratories by Dr. Peter A. Schultz of the Multiscale Dynamic Materials Modeling Department and collaborators. Using SeqQuest the tool enables users to calculate the total energy, atomic forces and stress for molecules, wires, slabs and bulk systems.
:seqQuest webpage

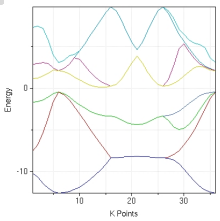
QC-Lab

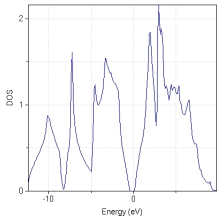


:powered by GAMESS
:QC-Lab – Quantum Chemistry Lab. It provides Ab Initio and DFT molecular and electronic structure calculations of small molecules.
:GAMESS Website

StrainBands



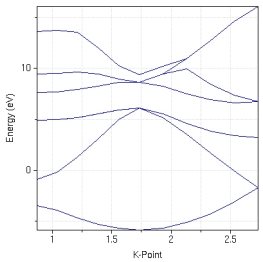


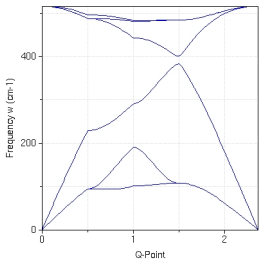


:powered by: Electronic structure calculations performed by ef5993a42152967>. Maximally-localized Wannier functions calculated by badf69eb100e2b>.

:This tool can be used to explore the influence of strain on first-principles bandstructures of semiconductors.

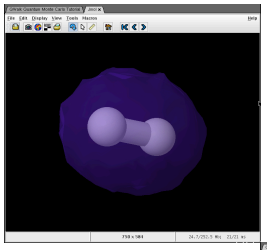
DFT calculations with Quantum ESPRESSO

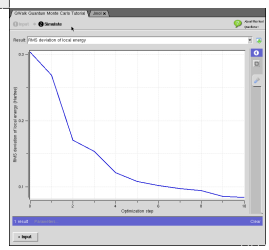




:This tool enables nanoHUB users to run quantum ESPRESSO, a powerful electronic structure code. Users can perform total energy calculations, energy minimization to predict structures, obtain the Kohn-Sham band structure of periodic systems as well as phonons.

[QWalk Quantum Monte Carlo Tutorial]

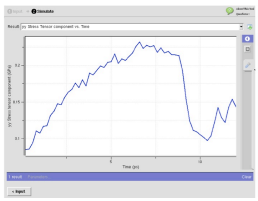
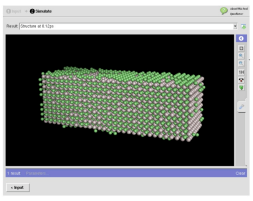




: Quantum Monte Carlo methods solve the Schrodinger equation for many electrons to high accuracy—exactly in some cases. In most implementations, it also has favorable scaling with system size, approximately the same as mean-field theories like density functional theory, although with a larger prefactor. This allows us to obtain accurate ground and excited state energies for realistic chemical systems. Quantities such as binding energies, reaction barriers, and band gaps are accurately simulated using QMC methods.
:qwalk Website

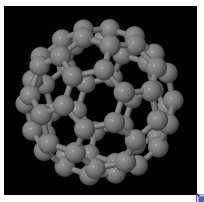
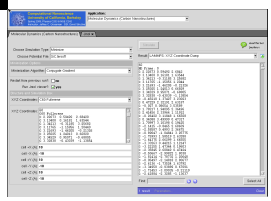
Molecular dynamics simulations Tools

[nano-Materials Simulation Toolkit]

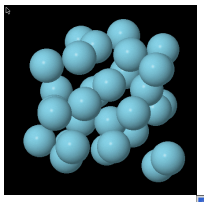
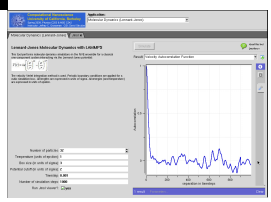

: powered b achan up MD
:The nanoM RIAL ulation toolkit enables users to perform molecular dynamics simulations of materials using a variety of force fields as well as electronic structure calculations.
:Atomic Picture of Plastic Deformation in Metals

LAMMPS for Carbon Nanostructures in MIT Atomic-Scale Modeling Toolkit

: powered by LAMMPS
:This tool is part of MIT Atomic-Scale Modeling Toolkit which serves Overview of Computational Nanoscience: a UC Berkeley Course
:LAMMPS Website

Lennard-Jones Potential with LAMMPS in MIT Atomic-Scale Modeling Toolkit

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:LAMMPS Website

Educational Material

Atomic Picture of Plastic Deformation in Metals is a Learning Module with Introductory Lectures, Tutorials and a Online-simulation Lab Assignment to the atomic-level processes responsible for plastic deformation in metals. Students will perform and analyze online molecular dynamics simulations and study.**Audience**: undegraduate and graduate students as well as instructors interested in mechanical response of materials.

Bonding and Bandstructure in Silicon is a Learning Module with Introductory Lectures, Tutorials and a Online-simulation Lab Assignment to explore how electronic bands form in Silicon and other materials. Students will perform online density functional theory calculations and explore the band structure and bonding of various materials. **Audience**: undegraduate and graduate students as well as instructors interested in electronic properties of materials.

Molecular dynamics simulations of materials is a topics page that summarizes educational resources and tools for molecular dynamics simulations.**Audience**: researchers interested in atomistic materials modeling and simulation.