Experiment No: 04

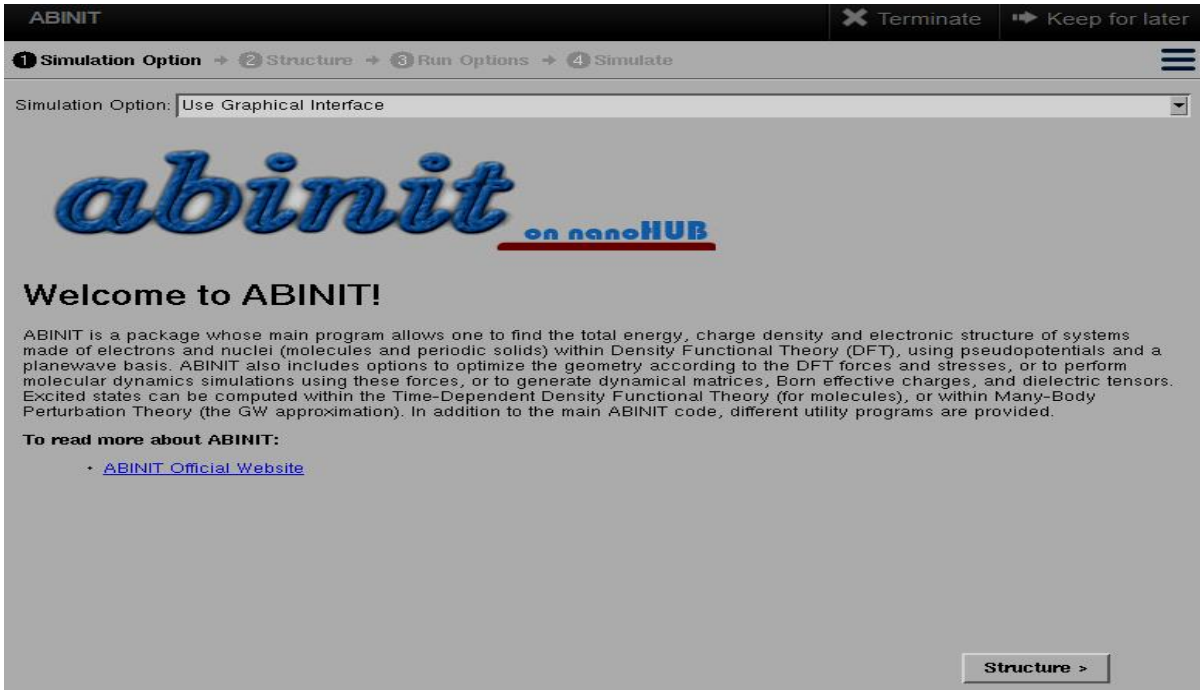
To test the performance of standard exchange- correlation functionals of DFT in determining structural properties of solids.

Abstract

To investigate the accuracy of standard exchange-correlations functionals in Density Functional Theory (DFT) calculations for determining structural properties of solids.Using ABINIT software, we test the Local Density Approximation(LDA), Generalized Gradient Approximation (GGA). The results shows that these exchange-correlation functionals yields lattice parameters closest to experimental values.These findings highlight the importance of functional choice in DFT calculations for PbO.

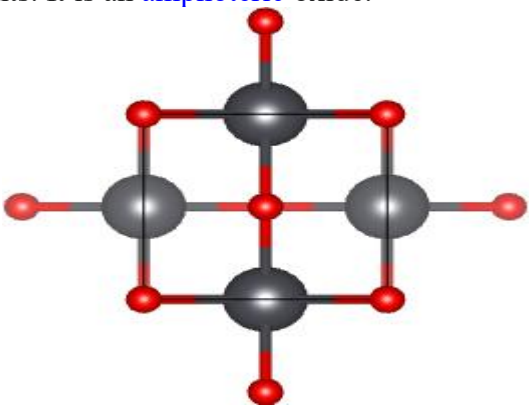
Introduction:

ABINIT is a package whose main program allows one to find the total energy, charge density, electronic structure and many other properties of systems made of electrons and nuclei, (molecules and periodic solids) within Density Functional Theory (DFT), Many-Body Perturbation Theory (GW approximation and Bethe Salpeter equation) and Dynamical Mean Field Theory (DMFT). ABINIT also allows to optimize the geometry according to the DFT forces and stresses, to perform molecular dynamics simulations using these forces, and to generate dynamical matrices, Born effective charges and dielectric tensors. The present paper aims to describe the new capabilities of ABINIT that have been developed since 2009. It covers both physical and technical developments inside the ABINIT code, as well as developments provided within ABINIT package.



Physical properties of Lead Oxide (PbO):

Lead(II) oxide, also called **lead monoxide**, is the inorganic compound with the molecular formula PbO. PbO occurs in two polymorphs: litharge having a tetragonal crystal structure, and massicot having an orthorhombic crystal structure. Modern applications for PbO are mostly in lead-based industrial glass and industrial ceramics, including computer components. It is an amphoteric oxide.



Chemical formula	PbO
Molar mass	223.20 g/mol
Appearance	red or yellow powder
Density	9.53 g/cm

Lattice type P
Space group name P 4/n m m
Space group number 129

Lattice parameters

a	b	c	alpha	beta	gamma
3.99000	3.99000	5.01000	90.0000	90.0000	90.0000

18 atoms, 16 bonds, 4 polyhedral

DFT properties of lead oxide

File type: **XYZ**

Coordinates type: Cartesian coordinates in angstroms

Scaling factor (x,y,z in bohrs): 9,9,4

Primitive lattice vectors:

a: 1, 0, 0 b: 0, 1, 0 c: 0, 0, 1

K-point setup: user defined array of k-points

Parameters:

No. of k-points; 4

K-points: (1, 4, 6)

K-point normalization: 1

Weights of k-points: 0.25do

Driver Parameters:

Exchange Correlation Functionls: LDA, GGA

Plane wave cutoff energy (har): 17.5

Dielectric constant: 25.9

Self consistent field (SCF) iterations

Self consistent algorithm: pulay mixing of density

Number of pulay iterations for SC mixing: 10

Convergence criterion for SCF iterations: Tolerance on difference of total energy

Parameters for SCF iterations

Number of self consistent iterations: 30

Target energy change (har): 1.0e -10

Band structure definitions

Band ranges to plot: (20, 35)

k- path specified by k points boundries: (1, 0, 0) (1, 0, 1)

Divison along k path between boundries: 6

Post processing

Wavefunction to visualize: (1, 0, 2) (1, 3, 6)

Execution via MPI:

Number of cores: 7

Hours: 1.5

Exchange correlations functionals

(LDA): Local-density approximations (LDA) are a class of approximations to the exchange–correlation (XC) energy functional in density functional theory (DFT) that depend solely upon the value of the electronic density at each point of space

(LDA) assumes variations of the density to be slow and treats the local density as a uniform electron gas

LDA uses the exchange for the uniform electron gas of a density equal to the density at the point where the exchange is to be evaluated,

$$E_x = \int d^3r\, n(\vec{r}) \left(\frac{-3e^2}{4\pi}\right) \left(3\pi^2 n(\vec{r})\right)^{\frac{1}{3}}$$

in SI units where $n(\vec{r})$ is the electron density per unit volume at the point $\vec{r}$ and e is the charge of an electron.

Generalized Gradient Approximation (GGA):

In the generalized gradient approximation (GGA) to DFT, the XC potential depends on the electron density ρ and its gradient ∇_ρ and is a complicated function in three-dimensional space.(GGA's), which incorporated density-gradient corrections to LSD, improve the agreement between calculated and measured energetics.

$E_{XC}^{GGA}[n] = \int V\varepsilon^{XLDA}(n(r\rightarrow))\ F_{XC}(n(r\rightarrow), \nabla n(r\rightarrow))d^3r$

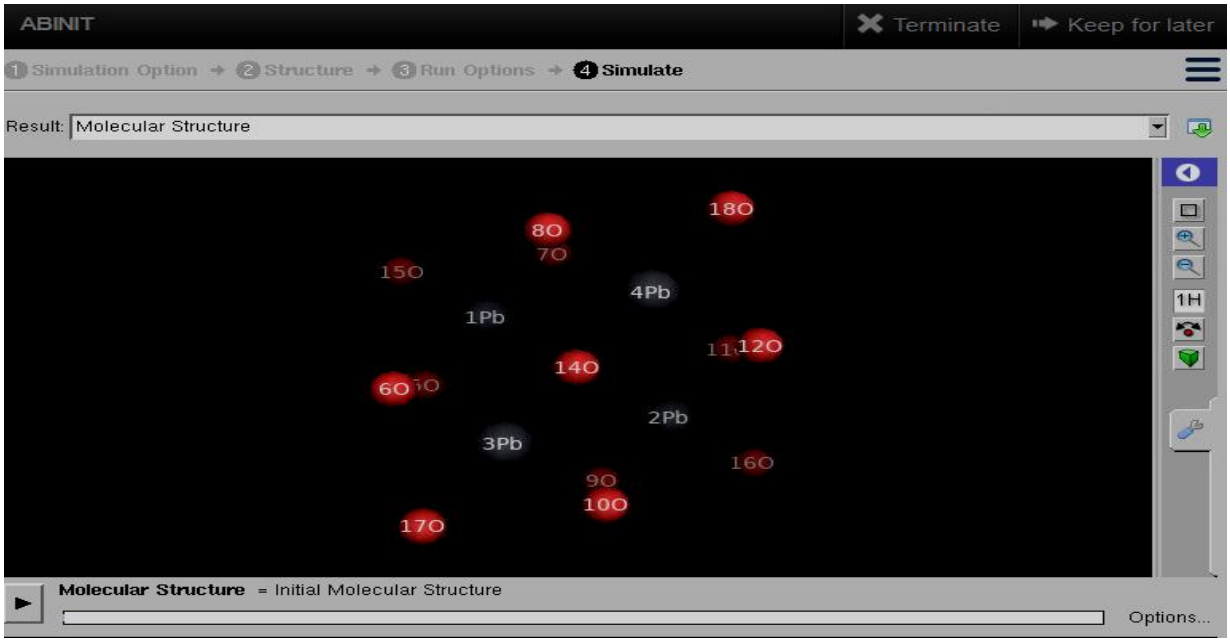
Materials and Methods

- XYZ file of PbO
- VESTA software for conversion of CIF file into XYZ file
- Laptop or computer

Methods:

- I launch the **ABINIT** software for DFT calculations.
- Then, open a XYZ file of Lead Oxide (PbO) generate from **VESTA** software in ABINIT software for input.
- I determined the PbO space group and lattice parameters from cif file used in VESTA software.
- Then I, provide specific values of PbO to ABINIT software for taking output.
- First, I open structure in menu bar of ABINIT software then change the values of all parameters which are present in this menu.
- Then I, open the driver parameters and give the suitable values of plane wave cutoff energy, dielectric constant, no. of pulay iterations and No. Of self consistent (SC) iterations.
- Similarly I provide all suitable values for all parameters present in Bandstrcture menu, post processing menu and then Run options.
- Then, I simulate all input through simulate option in the menu bar of the software.
- I, also calculate the exchange correlation functionals (LDA, GGA) one by one.
- Finally I determined the output results of PbO for DFT calculations

Lab View



Observations

Exchange correlations	k-points	Weights of k-points	Cutoff-energy
LDA	4	0.25	17.5
GGA	6	1.0	24.9

Output

Abinit Inputdeck

Number of Data Sets
(Ndtset) 2
Definition of the unit cell
A cell scalng factor 9 9 4
Reciprocal path integration method (rprim) 1 0 0
0 1 0
0 0 1

Definition of the atom types
Number of tyoes of atoms (ntypat) 2
Atomic nuclear charge (znucl) 82 8

Iterations foe exchange correlation functionals (ixc) 1
Definition of the atoms
Number of atoms (natom) 18
Type of atomic index (typat) 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2

Definition of the planewave basis set
Cutoff energy (ecut) 17.5

Definition of the SCF procedure
Number of steps for convergence (nstep) 30
Tolerance on difference of total energy (toldfe)1 1.0e-10
Dielectric constant (diemac) 25.9
Usual self-consistent calculation
Kpoint option (kptopt) 1 1
Print density (prtden) 1 1
Bandstructure Calculations
Iterative self consistent field (iscf) 2 -2
Get density (getden) 2 -1
K point options (kptopt) 2 -1
Print eigenvalues (prteig) 2 1
Print volume (prtvol) 2 3
Number of bands (nband) 2 35

Conclusion:

The study investigated the performance of various standard exchange- correlations functionals (LDA,GGA) within DFT in predicting structural properties of solids.LDA underestimates lattice constant while GGA overestimate them.

References:

M. Y. chern et,.Jphys; condense. Matter 27.035501
U. Schroder etal,. Jphys;. condense. Matter 29,445501