Experiment No: 05

To determine the preferred crystal structure of an element solid using DFT calculations and comparing results with available literature.

Abstract:

Employed DFT calculations to investigate the crystal structure of Silicon dioxide (SiO2). Using the LDA (Local- density approximation) functional and plane wave basis sets, optimized the structural parameters, lattice constants, and bond lengths of SiO2. DFT calculations accurately reproduce the structure of SiO2, validating the computational approach.Preliminary results shows that SiO2 structure parameters are consistent with experimental and theoretical values.

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

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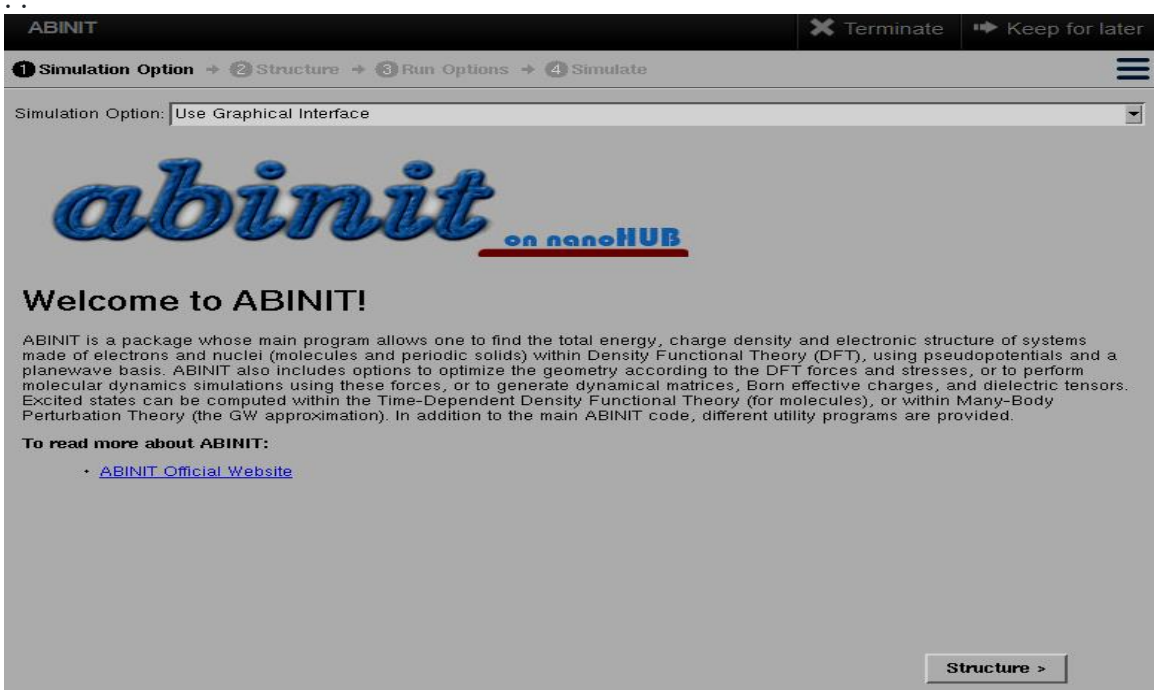
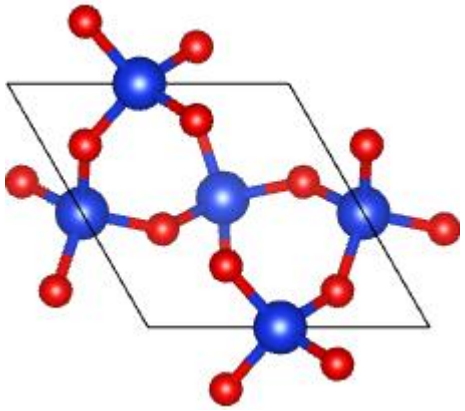


Properties of Silicon dioxide (SiO2):



SiO2 is an oxide of silicon with a chemical name silicon dioxide. It is also called Silica or Kalii bromidum or Silicic oxide or silicic acid. It is widely found in nature as **quartz.**It is obtained as a transparent to grey, in its crystalline or amorphous powdered form. It is odourless and tasteless compound.

Molecular weight of SiO2	60.08 g/mol
Density of Silicon dioxide	2.648 g/cm3
Melting point of Silicon dioxide	1,713 °C
Boiling point of Silicon dioxide	2,950 °C

Lattice type C
Space group name Custom
Space group number 154
Setting number 1

Lattice parameters

a	b	c	alpha	beta	gamma
4.91000	4.91000	5.40000	90.0000	90.0000	120.0000

Unit-cell volume = 112.742421 Å^3

The complex structure and the presence of Oxygen atoms conspire to make a first-principles theoretical study of SiO2 especially difficult. Recently, with the help of newly developed fast iterative algorithms for DFT calculations e.g ABINIT software, SiO2, successfully studied using pseudo-potential density functional plane- wave methods. However, the use of conventional norm- conserving oxygen pseudo potentials in these studies requires a relatively large plane- wave cutoff, rendering this approach problematic for more studies on complex systems involving defects,

surfaces and disorders. A more efficient approach has recently been developed which combines the use of a separable pseudopotential by pulay mixing of potential algorithm. This method has successfully been applied to study applications as diverse as phase transitions of SiO2. In this report, present an application of this method for SiO2 using ABINIT software. A psuedopotential has been generated for Oxygen to correctly predict the energetics and the structural properties with a plane wave cutoff ranges are **25 - 40 R_Y**.
SiO2 has been one of the most extensively studied materials due to its application potential in ceramic and glass industries as well as in optical fibers, microelectronics and catalysis. On the other hand, it is also one of the most difficult material to study. Because of the difficulties only a few crystal- line structures of SiO2 have been investigated with first- principles techniques, although the complex bonding situation in silica with a mixture of ionic and covalent interactions speaks to the necessity for a treatment on an ab- initio microscopic level.In the present study, carried out an extensive study to calculate the energetics and structural parameters of SiO2.
The fact that use a uniform theoretical treatment facilitates systematic comparisons and identification of SiO2.

File type: XYZ Coordinates type: Cartesian coordinates in angstroms

Scaling factor (x,y,z in bohrs): 0.95,0.95,1.05

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: (4, 4, 4)

K-point normalization: 1

Weights of k-points: 0.375do

Driver Parameters:

Exchange Correlation Functionls: LDA

Plane wave cutoff energy (har): 25

Dielectric constant: 4.6

Self consistent field (SCF) iterations

Self consistent algorithm: pulay mixing of potential

Number of pulay iterations for SC mixing: 6

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: (17, 31)

k- path specified by k points boundries: (1, 0, 0.5) (1, 0, 1)

Divison along k path between boundries: 2

Post processing

Wavefunction to visualize: (1, 2, 4) (1, 1, 3)

Execution via MPI:

Number of cores: 3

Hours: 1.0

In most cases, K-point sampling has converged at about 0.002ev/atom on going to the next higher k- point set.

Materials and Methods:

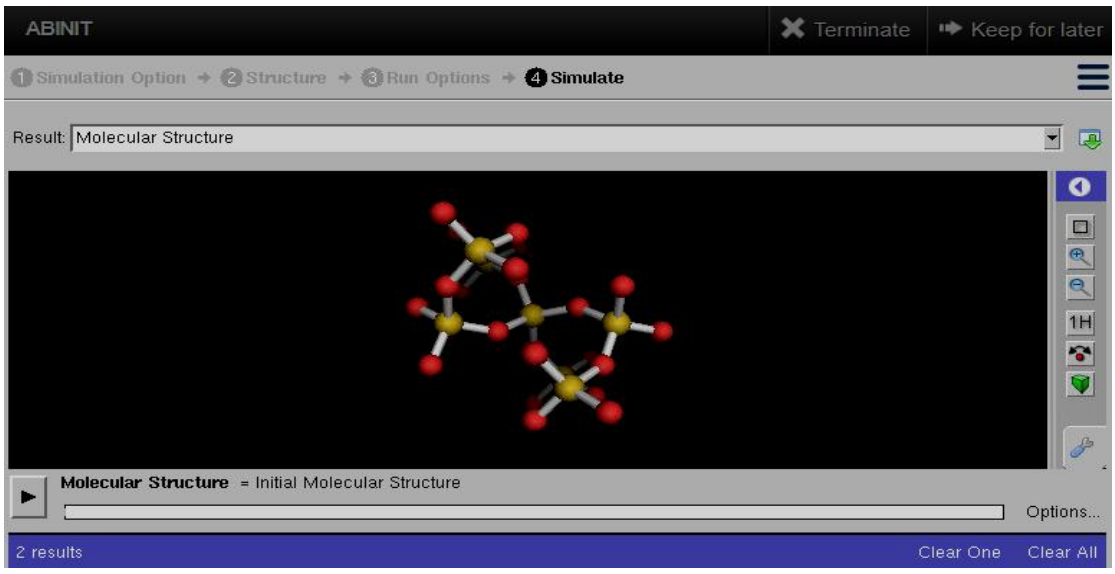
- XYZ file of SiO2
- VESTA software for conversion of CIF file into XYZ file
- Laptop or computer

Methods:

- I launch the **ABINIT** software for DFT calculations.

- Then, open a XYZ file of SiO2 (silicon dioxide) generate from **VESTA** software in ABINIT software for input.
- I determined the SiO2 space group and lattice parameters from cif file used in VESTA software.
- Then I, provide specific values of SiO2 to ABINIT software for taking output.
- Firstly 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
- Finally I determined the output results of SiO2 for DFT calculations especially cutoff energy and K-points
- I used LDA functional and collect the data for 2 simulations, then compare it with available literature of SiO2.
- I also draw a graph between cutoff energy values and k-points values.

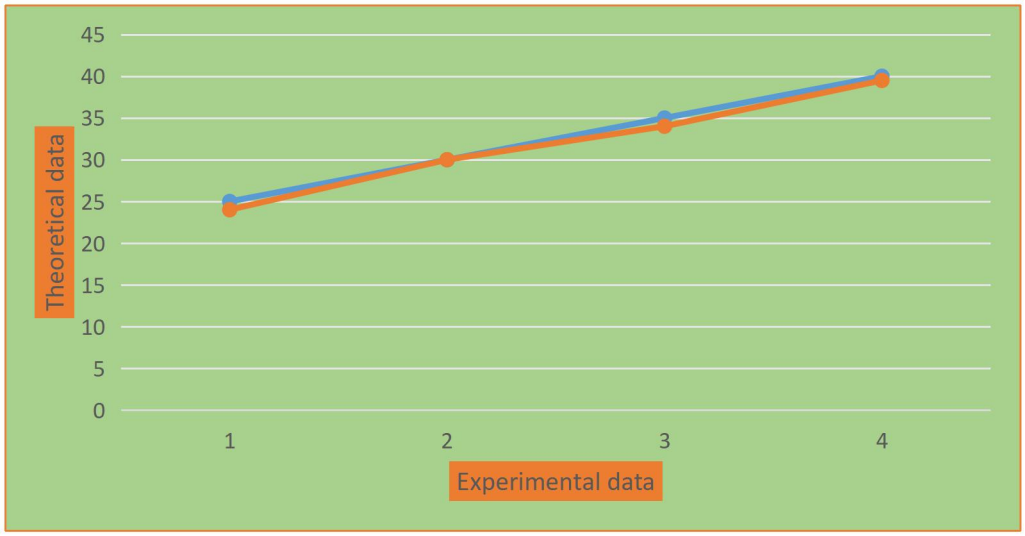
Lab view:



Observations:

Lattice parameters	Theoretical	Experimental
4.26	25.00	24.01
4.27	30.00	30.002
4.29	35.00	34.01
4.31	40.00	39.5

Analysis:



Output:

#abinit inputdeck

Definition of the unit cell
Scaling factor (acell) 0.95 0.95 1.05
Reciprocal Primitive lattice vector (rprim) 1 0 0
0 1 0
0 0 1

Definition of the atom types
Number of types of atoms (ntypat) 2
Atomic nuclear charge (znucl) 14 8

Definition of the planewave basis set
Plane wave cutoff energy (ecut) 25

Definition of the k-point grid
Kpoint option (kptopt) 0
No of k-points (nkpt) 4
K-ponits (kpt) 4, 4, 6
Norm of the k-points (kptnrm) 1
Weights of k-points (wtk) 0.375d0

Ion movement (ionm) ov 0
opt-cell 0
Definition of the SCF procedure
Self consist field algorithm (iscf) 7
No of pulay mixing (npulayit) 6
 Maximum no of iterations (nstep) 30
Tolerance on the difference of total energies (toldfe) 1.0e-10
Dielectric constant (dimec) 4.6

Conclusion:

Finally, demonstrate that the use of pseudo-potentials make it possible to obtain accurate results, using a plane wave cutoff energy ranges are 25- 40 Ry. Since the best that has been achieved with norm- conserving oxygen pseudo-potentials is 40Ry, the present method shows great promise of future applications. I use equivalent k-point sampling as much as possible for SiO2 structure to make parallel comparison in energy values.

References:

1. A research paper of “First- principle study of crystalline silica”
2. Phys. Rev. B 84, 045207 (2011)