Available online www.jocpr.com

Journal of Chemical and Pharmaceutical Research, 2015, 7(7):289-291

Research Article

ISSN : 0975-7384
CODEN(USA) : JCPRC5

First principle study of phase transition in CaO

N. Munjal[1*], K. Bhakri[1] and G. Sharma[2]

[1]School of Physical Sciences, Lovely Professional University, Jalandhar-Delhi, Phagwara, Punjab, India
[2]Department of Pure & Applied Physics University of Kota, Near Kabir Circle, Kota, Rajasthan, India

---

ABSTRACT

As a quantum mechanical function describes all the information about the system. We can solve the Schrodinger wave equation for a 2- body system or hydrogen atom to determine the allowed energy states of the system by knowing its wave function, but it is not possible to solve the Schrodinger wave equation for a N- body system. So the ultimate solution for this is the DFT. In the present work, the linear combinational of atomic orbital method as embodied in CRYSTAL code have been used to investigate the phase transition in technologically important compound CaO. The correlation and exchange scheme of PBE and Becke is used for building the Kohn-Sham Hamiltonian.

Keywords: LCAO, DFT, HF, CRYSTAL, PBE, Becke, CaO

INTRODUCTION

The rare-earth elements have drawn great interest, both theoretically as well as experimentally due to their remarkable semi conducting properties and they have lots of relevance in an area of non-linear optics, glass-making electro-optic parts, breaking alloys etc. These elements are the part of green technological industry. The 2nd group elements containing Mg, Be, Ba Sr, Ca, Sr, Ra are called as alkaline earth elements. These elements are soft and almost silver in color with low boiling and melting points. They are having relatively low densities. The second group elements have just 2 electrons in their outermost shell so they have second-lowest first ionization energy with respect to other groups in the periodic table. These alkaline earth elements react with oxygen to form oxides (CaO, MgO, SrO..etc). Due to their abundance in earth's mantle, oxides of Mg and Ca are widely investigated experimentally and theoretically and found to have wide band gaps. These oxides are having several technological and industrial uses ranging from catalysis to microelectronics [1]. CaO shows high mechanical resistance and radiation resistance, and it has wide energy band gap of the order of 7.1 eV with a high value of dielectric constant i.e. 11.8 [2]. CaO is used many bio-medical applications like biosensors. It can play a vital role in the field of spintronics [3,4]. Since, magnesium oxide has large band gap (~7.833eV) and dielectric constant [2], so it is used in industrial sciences high dielectric constant, and can easily form ternary phases.

This work is focused on the investigation of phase transition in CaO by using LCAO approach as present in Crystal code [5].

Structural parameters of CaO has been described and studied by many researchers both theoretically and experimentally [6-16]. The periodic *ab-initio* LCAO method have been employed by Habas et al [6] to study the structural parameters of B1 and B2 phases of alkaline earth oxides including MgO and CaO. They applied HF and DFT schemes. The electronic structures of MgO and CaO have been performed by Baltache et al [7] using FP-LAPW method. They have used LDA for exchange and correlation potentials. The ground state properties of CaO is being studied by Deng et al [8] with the use of *ab-initio* PW-PP method as present in CASTEP code.The bonding in MgO and CaO has been studied by Israel et al [9] using maximum entropy method. Medeiros et al [10] have performed a theoretical study on structural parameters of CaO using ABINIT code. They have used both LDA and

GGA schemes. The structural and electronic properties of CaO have been investigated by Ghebouli et al [11] using the DFT as embodied in CASTEP code. Srivastava et al [15] studied phase transformation in CaO by the use of first-principles DFT and charge transfer interaction potential method. Experimentally, the different parameters of CaO have explored by Jeanloz and Ahrens [16]. They have used shock wave and diamond cell experiments.

EXPERIMENTAL SECTION

In the present work, the phase transition in CaO is calculated by solving the Kohn Sham equations under the DFT [17] as present in CRYSTAL [5] code. The code is developed by the researchers of the Theoretical Chemistry group in Torino (Italy) and the Computational materials sciences group in CLRC (Daresbury, UK) developed a very useful and efficient code with lots of scientific importance in 1978.The CRYSTAL program calculates the electronic as well as the structural properties of periodic systems in the context of HF [18], DFT and several hybrid estimates. "*CRYSTAL is a program for exploring the crystalline solids."* This code can be referred to accomplish investigations of the chemical and physical properties of crystalline solids, polymers, molecules, nanotubes etc. It can also compute the vibrational, magnetic piezoelectric, elastic, dielectric and photo elastic properties of any type of compounds. This method has given excellent results for many compounds [19-21].

For Ca and O, the local functions were built from the basis sets of Gaussian [22]. The K-S Hamiltonian has been build while considering exchange scheme of Becke [23] and PBE [24] correlation scheme. The 165 **k** pints were used with adequate tolerance. The 45 % mixing and within the 15 cycles the self-consistency is attained.

RESULTS AND DISCUSSION

The Gibbs free energy ($G = E_o + PV - TS$) is used for calculating the transition pressure. Since all our density functional calculations are conducted at T = 0 K, the Gibbs free energy reduces to the enthalpy, $H = E_o + P V$. At a particular pressure, the thermodynamically stable phase is that whose enthalpy has the smallest value. The transition from one phase to the high pressure phase takes place when the enthalpy curves coincides. For CaO, transition from B1 to B2 occurs at 48.5 GPa. Comparison of present calculated values along with previous calculations is presented in Table 1.

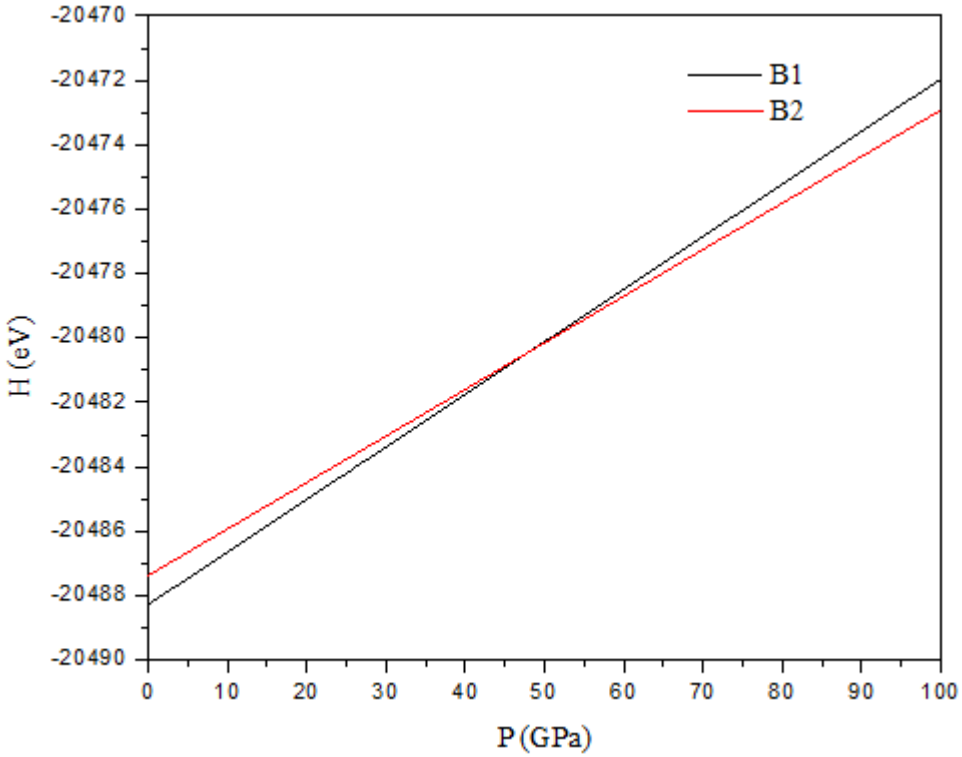

Figure 1. Enthalpy versus pressure curve for CaO

Table 1: Transition Pressure in GPa

	Present	Experimental	Other Calculations
CaO	48.5	60 ± 10 [16]	63 [12], 55 [13], 54.2 [14], 56 [15]

CONCLUSION

In summary, the structural B1(NaCl)–B2(CsCl) phase transition of CaO is investigated by the LCAO method. It is found that the B1–B2 structural transformation occurs at about 48.5 GPa which is in little bit underestimated than the earlier calculations.

REFERENCES

[1] RC Whited; CJ Flaten; WC Walker, *Solid State Commun*., **1973**, 13(11), 1903-1905.
[2] A Dorner-Reisel; C Schurer; C Nischan; O Seidel; E Muller, *Thin Solid Films,***2002**, 420-421, 263-268.
[3] DV Sthtansky; EA Levashov; NA Glushankova; NB D'yakonova; SA Kulinich; MI Petrzhik; FV Kiryukhantsev-Korneevand; F Rossi, *Surf. Coat. Technol.,* **2004,**182(1), 101-111.
[4] Y Fujiwara; T Isobe; M Senna; J Tanaka, *J. Phys. Chem. A.*,**1999,** 103(48), 9842-9846.
[5] R Dovesi; VR Saunders; C Roetti; ROrlando; CM Zicovich-Wilson; F Pascale; B Civalleri; K Doll; NM Harrison; IJ Bush; Ph D'Arco; M Llunell, CRYSTAL06 User's manual(University of Torino, Torino)**2006**.
[6] MP Habas; R Dovesi; A Lichanot, *J. Phys. Condens. Matter,***1998** 10(31), 6897.
[7] H Baltache; R Khenata; M. Sahnoun, M. Driz; B. Abbar; B Bouhafs, *Physica B.*,**2004** 344(1-4), 334.
[8] Y Deng; OH Jia; XR Chen; J Zhu, *Physica B.*,**2007**, 392(1-2), 229.
[9] S Israel; R Saravanan; N Srinivasan; SK Mohanlal, *J. Phys. Chem. of solids,***2003**, 64(5), 879.
[10] SK Medeiros; EL Albuquerque; FF Maia; EWS Caetano; GA Farias; VN Freiere; BS Cavada; ML Pessati; TLP Pessati, *Microelectronics Journal,***2005** 36(11), 1058-1061.
[11] B Ghebouli; MA Ghebouli; M Fatmi; M Benkerri, *Material Science in Semiconductor Processing*, **2010**, 13(2), 92-101.
[12] JF Mammone; HK Mao; PM Bell, *J. Geophys. Res. Lett.,* **1981,** 8, 140-142.
[13] MJ Mehl; RJ Hemley; LL Boyer, *Phys. Rev. B.,* **1986**33(12-15), 8685.
[14]MJ Mehl; RE Cohen; H Krakauer, *J. Geophys. Res.,* **1988**93, 8009.
[15] A Srivastava; M Chauhan; RK Singh; R Padegaoner, *Phys. Status. Solidi B.*, **2011** 248(8), 1901-1907.
[16] R Jeanloz; TJ Ahrens, Geophys. *J. R. Astron. Soc.*,**1980,** 62, 505.
[17] R Dovesi; R Orlando; C Roetti; C Pisani; VR Saunders, *Phys. Status Solidi B.*,**2000,**217(1)**,**63-68.
[18] C Pisani; R Dovesi; C Roetti;Hartree–Fock. Ab InitioTreatment of Crystalline Solids(Lecture Notes in Chemistry vol. 48) Springer,Heidelberg,**1988**.
[19] R Kumar;N Munjal; V Vyas; GSharma; MS Dhaka; BK Sharma, *Phase Transition*, **2012**, 85(12), 1098-1108.
[20**]** N Munjal; G Sharma; V Vyas;KB. Joshi; BK Sharma,*Phil. Mag.*,**2012,** 92(24), 3101.
[21] N Munjal; V Sharma; G Sharma; V Vyas; BK Sharma; JE Lowther,*Phys. Scr.*,**2011**, 84(3), 035704.
[22] www.tcm.phy.cam.ac.uk.
[23] AD Becke, *J. Chem. Phys*.,**1993,** 98(7),5648-5652.
[24] JP Perdew; K Burke; M Ernzerhof,*Phys. Rev. Lett*.,**1996** 77, 3865.