Journal of Physical and Theoretical Chemistry
of Islamic Azad University of Iran, 8 (3) 199-204: Fall 2011
(J. Phys. Theor. Chem. IAU Iran)
ISSN 1735-2126

AB Initio Study of Molecular Struture, Energetic and Vibrational Spectra of $(GaN)_4$ Nanosemiconductor

E. Pournamdari[1*] and M. khaleghian[2]
[1] Ph.D. Student, Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran
[2] Department of Chemistry, Islamshar Branch, Islamic Azad University, Tehran, Iran

Received November 2011; Accepted November 2011

ABSTRACT

In recent years there has been considerable interest in the structures, energies and thermodynamics of $(GaN)_4$ clusters and it is the subject of many experimental and theoretical studies because of their fundamental importance in chemical and physical process. All calculation of this study is carried out by Gaussian 98. Geometry optimization for $(GaN)_4$ nanocluster are be fulfilled at B3LYP, BlLYP and LSDA levels of theory with LANL2DZ basis set. Calculated are accomplished at 298 K. The structures, energetic and thermodynamic properties and vibrational spectra will be discussed.

Keywords: Nanocluster; Semiconductor; Ab Initio; IR, Vibrational Frequencies; Structure; Energetic

INTRODUCTION

Recent progress in the synthesis and characterization of one-dimensional nanostructures has been driven by the need to understand the novel physical properties of one-dimensional nanoscale materials, and their potential application in constructing nanoscale electronic and optoelectronic devices [1]. Group III–V semiconductors are promising materials because of the potential applications in optical communications and full colour displays. GaN is a wide and direct band-gap semiconductor, which exhibits less thermal quenching and stronger RE emission at room temperature [2]. The wide-band-gap semiconductor GaN is currently of great interest for development of optoelectronic devices at blue and near-ultraviolet wavelengths as well as high-temperature and -frequency electronics, such as violet light emitting diodes (LEDs). The one-dimensional GaN semiconductor nanostructures are electronic confines systems ideal for fundamental studies of their physical properties and for the fabrications of new optoelectronic nanodevices [3]. Over a past decade, different high performance devices systems with nitride material have been concentrated for intense research [4–6]. These materials represent wide band gaps in the ultraviolet (UV) and visible (VIS) range, i.e. Eg (eV) =6.2 (AlN), 3.4 (GaN) and 1.9 (InN) [7]. Current GaN-based device technologies include light-emitting diodes (LEDs), laser diodes and UV detectors on the photonic side and microwave power and ultra-high power switches on the electronics side [8].

The applications for GaN-based devices include displays and data storage, solar-blind UV detectors, new sensor technologies, wireless communications, solid-state lighting and high power microwave generation for radar [9]. In order to growth of GaN and relative semiconductors

* Corresponding author: E. Pournamdari

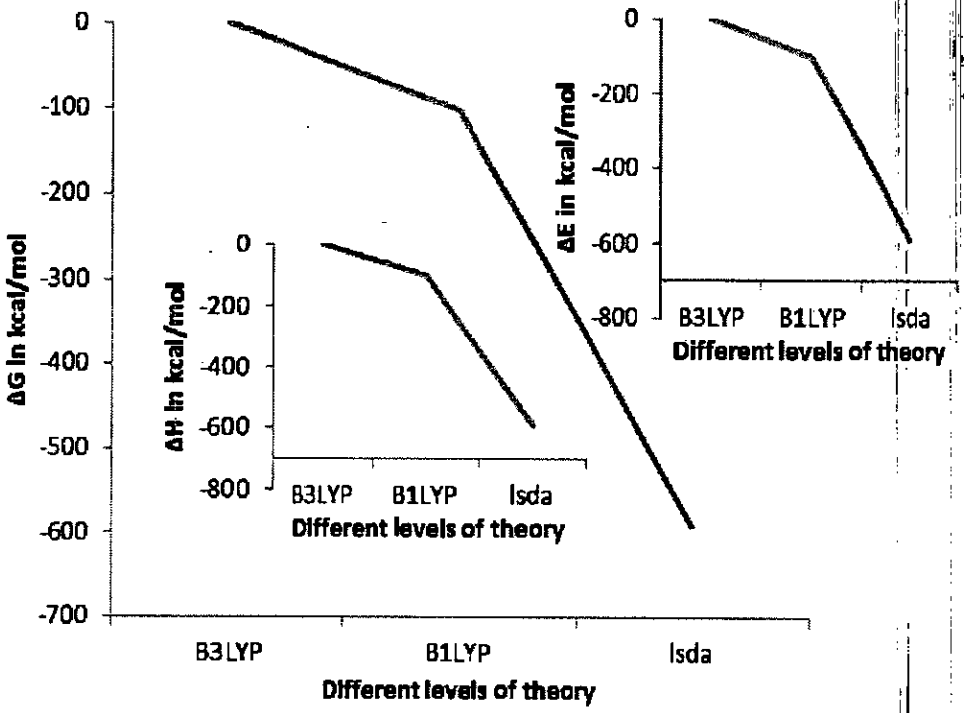

Fig. 2. Different levels of theory as a function of ΔG, ΔH, ΔE in kcal/mol.

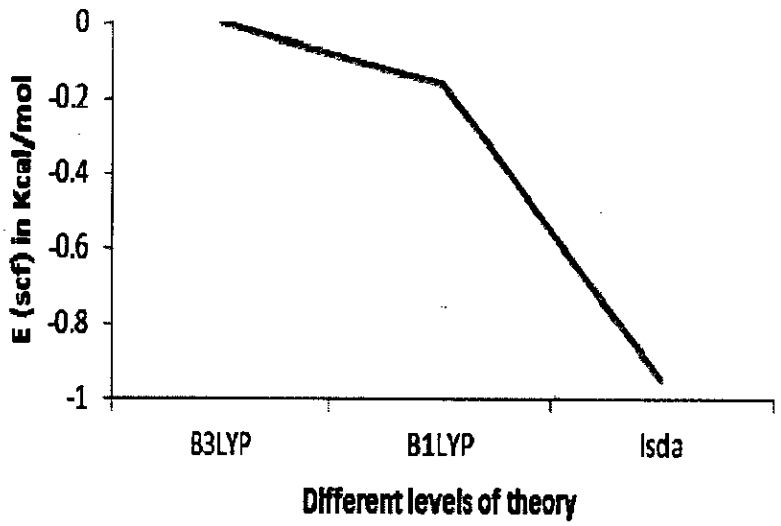

Fig. 3. Different levels of theory as a function of energy (scf) in kcal/mol.

Vibrational spectra

Frequency and IR intensities of $(GaN)_4$ nanosemiconductor cluster are calculated with B3LYP, B1LYP and LSDA methods using LANL2DZ basis sets and IR spectrum of this nanocluster shown in fig. 4, 5, 6 for B3LYP, B1LYP and LSDA methods of density functional theory (DFT), respectively. As can be seen the maximum intensity in B3LYP levels of theory is at frequencies of 486.812 cm^{-1} with 160.736 intensities, for B1LYP is at frequencies of 485.494 cm^{-1} with 162.834 intensities and for LSDA levels of theory is at frequencies of 492.57 cm^{-1} with 139.749 intensities. LSDA method has largest blue shift in

comparison of B3LYP and B1LYP levels of theory.

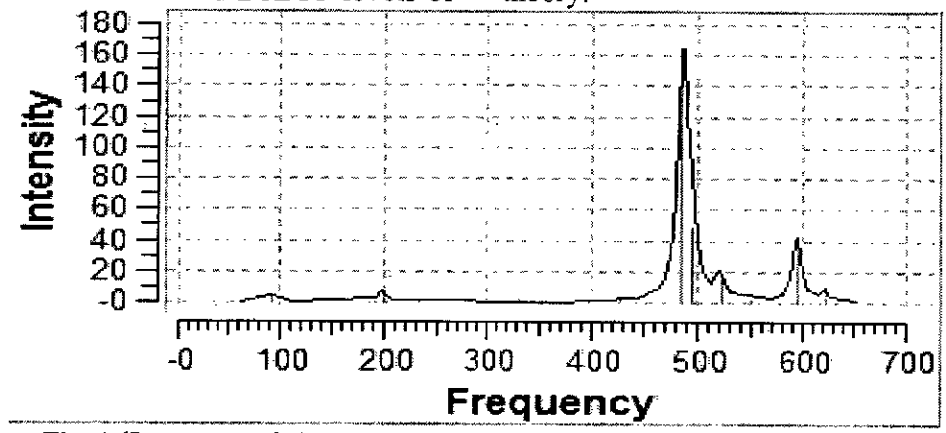

Fig. 4. IR spectrum of $(GaN)_4$ system obtained from B3LYP/LANL2DZ methods.

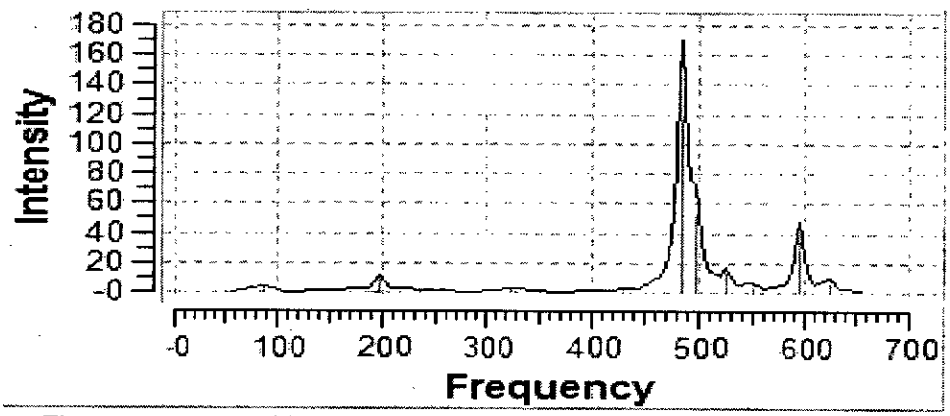

Fig. 5. IR spectrum of $(GaN)_4$ system obtained from B1LYP/LANL2DZ methods.

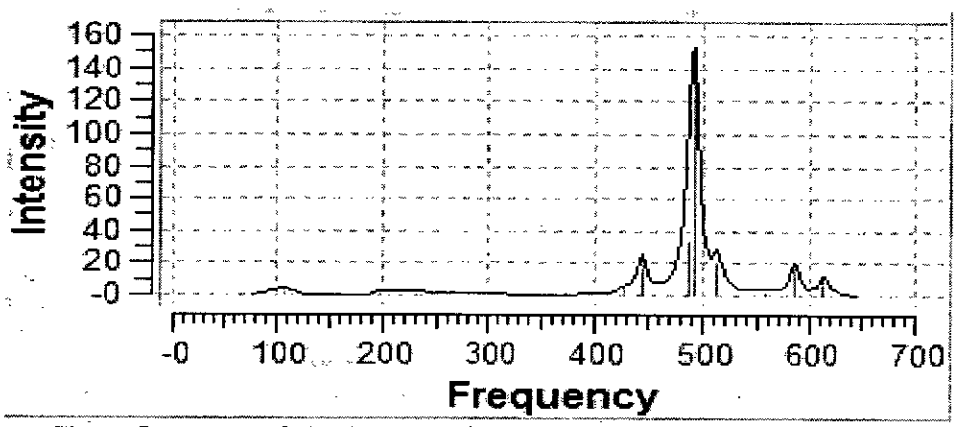

Fig. 6. IR spectrum of $(GaN)_4$ system obtained from LSDA/LANL2DZ methods.

REFERENCES

[1] J. T. Hu, T.W. Odom and C. M. Lieber, Acc. Chem. Res., 32 (1999) 435.

[2] P. N. Favennec, H. L'Haridon, M. Salvi, D. Moutonnet and Y. Le Guillou, J.Electron. Lett., 25 (1989) 718.

[3] T. P. Chow, R. Tyagi and IEEE Trans. Electron. Devices, J. 41 (1994) 1481.

[4] Y. F. Wu, B. P. Keller, S. Keller, D. Kapolnek, P. Kozodoy, S. Denbaars and U.K. Mishra, J. Appl. Phys. Lett., J. 69 (1996) 1438.

[5] R. J. Trew, M.W. Shin, V. Gatto, J. Solid-State Electron, 41 (1997) 1561.

[6] R. Gaska, M. S. Shur, A. D. Bykhovski, A.O. Oriov, G.L. Snider, J.Appl. Phys. Lett., 74 (1999) 287.

[7] (a) G. P. Pomrenke, P. B. Klein, D. W. Lange (Eds.), Mater. Res. Soc. Symp. Proc. MRS, Pittsburgh, PA., 301(1993). (b) S. Cotta, A. Polman, R.N. Schwartz (Eds.), Mater. Res. Soc. Symp. Proc. MRS, Pittsburgh, PA., 422 (1996).

[8] See for example GaN and Related Materials, ed. S.J. Pearton (Gordon and Breach, NY, (1997) and GaN, ed. J.I. Pankove and T. D. Moustakas (Academic Press, San Diego 1988), and references therein.

[9] SJ. Pearton, J.C. Zolper, RJ. Shul and F.Ren " GaN: DEFECT AND DEVICE ISSUES ".

[10] Ve´zian, S.; Le Louarn, A and Massies, J. J. Cryst. Growth., 303 (2007) 419.

[11] Meng, G.; Liu, X.; Xie, S. and Peng, D. J. Cryst. Growth., 232 (1996) 163.

[12] Yang, Y.-G.; Ma, H.-L.; Xue, C.-S; Hao, X.-T.; Zhuang, H.-Z and Ma, J. Physica, B325 (2003) 230.

[13] Xue, C.; Yang, L.; Wang, C.; Zhuang, H. and Wei, Q. J.Appl. Surf. Sci.153 (2003) 210.

[14] Dadgar, A.; Schulze, F.; Wienecke, M.; Gadanecz, A.; Bla¨sing, J;. Veit, P.; Hempel, T.; Diez, A.; Christen, J.and Krost, A. New J. Phys., 389 (2007) 9.

[15] Takemoto, K.; Murakami, H.; Iwamoto, T.; Matsuo, Y.; Kangawa, Y.; Kumagai and Y.; Koukitu and A. Jpn, J. Appl. Phys. 45 (2006) L478.

[16] Naritsuka, S.; Kondo, T.; Otsubo, H.; Saitoh, K.; Yamamoto, Y and Maruyama, T. J, Cryst. Growth, 300 (2007) 118.

[17] Ishikawa, H.; Yamamoto, K.; Egawa, T.; Soga, T.; Jimbo, T;. Umeno and M. J, Cryst. Growth 189/190 (1998) 178.

[18] Wu, Y.; Xue, C.; Zhuang, H.; Tian, D.; Liu, Y.; He, J.; Wang, F;. Sun, L. and Ai, Y. Mater, J. Lett, 60 (2006) 3076.

[19] Ji, X. H.; Lau, S. P.; Yang, H. J. and Zhang, Q. Y, J. Thin Solid Films.515, (2007)4619.

[20] Chang, K. J.; Chang, J. Y.; Chen, M. C.; Lahn, S. M.; Kao, C. J;. Li, Z. Y.; Uen, W. Y.; Chi, G. C; J. Vac. Sci. Technol. 25 (2007) 701.

[21] Yodo, T.; Shimada, T.; Tagawa, S.; Harada, Y, J. Cryst. Growth. 301-302, (2007), 504.

[22] Gaussian 98, Revision A.7, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr,.R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi,V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi ,R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 1998.

[23] Check C. E., Faust T. O., Bailey J. M., Wright B. J., Gilbert T. M. and Sunderlin L. S., J. Physical Chemistry A, 105 (34), (2001) 8111.

[24] Parlak C, J. Molecular Structure, 966 (1-3) (2010) 1.

[25] Hay P.J. and Wadt W.R., J. Chem. Phys 82 (1) (1985) 270.