



Vibratory Properties of SiP & Nanocrystals, Depending on Size by Using Infrared Spectroscopy via Density Functional Theory

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Shahd khaled mohammed¹

Bilal K. Al-Rawi²

^{1,2} Physics Department, Anbar University

Abstract

Actually, Raman spectra and infrared radiation along with Density Functional Theory (DFT) are used at the PBE/ 6-31G level including polarization functions to get vibratory properties of silicon phosphide crystal (SiP).

Therefore, several physical properties, including energy gaps, tetrahedral angles, and dihedral angles, have been studied.

On one hand, all the results showed a decrease in the energy gap with an increase in size that starts from Diamamentan, Tramamentan, Hexamamentan and Octamentan. It then recorded the longest bond at 1.91Å in Diamamentan. On the other hand, the tetrahedral angles of Tramamentan and Hexamamentan recorded a value of 109° as well as they are much closer to the ideal value of 109.43°. In addition to Infrared Radiation and Raman spectra were found as a vibratory frequency function.

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Introduction

In fact, controlling the physical and visual properties of nanoparticles is important. Moreover, Infrared spectrometry is a good strategy to study the focus of free carriers on semiconductor materials. The concentration of free carriers of SiP nanoparticles is studied using hydrogen [1]. Theoretical calculations of vibratory infrared oscillations and Raman spectra of the nanocrystal group made of SiP and the difference in these vibrations from molecular size to mass size, carried out earlier [2]. Full geometric optimization calculations are available for execution with (DFT) in Gaussian 0.9 program [3]. Current work is concerned with theoretical calculations of the vibratory infrared frequency lines of nano-crystals diamond with (SiP) as well as the difference in these vibrations from molecular to mass size [4]. These differences in different properties from molecule to nano are important to understand how these materials are handled in the field of nanotechnology [5].

Theory

Density Functional Theory (DFT) has used for generalized-gradient approximation (GGA) and base group PBE/ 6-31G (d) containing polarization functions. Engineering improvement is performed first followed by frequency and vibration analysis [6]. All calculations made using Gaussian 0.9 program to improve molecular vibration [7].

Results & Discussion

When base groups PBE/ 6-31G (d) are used, the power gap decreases from 4.9 eV in SiP for Diamamentan to 4.35 eV in SiP for Octamentan. A decrease in this energy relates returns to imprisonment effects that require reducing the size of the energy gap as shown in Figure (1). As it noted in Figure (2), the smallest energy gap recorded at 4.35 eV in SiP for Octamentan. When the mentioned base group is used, negative values appear in both the highest and lowest occupied and unoccupied molecular orbits (HOMO, LUMO); these indicate that additional energy is needed to extract the electron from the molecular or add the electron, making such structures very stable.



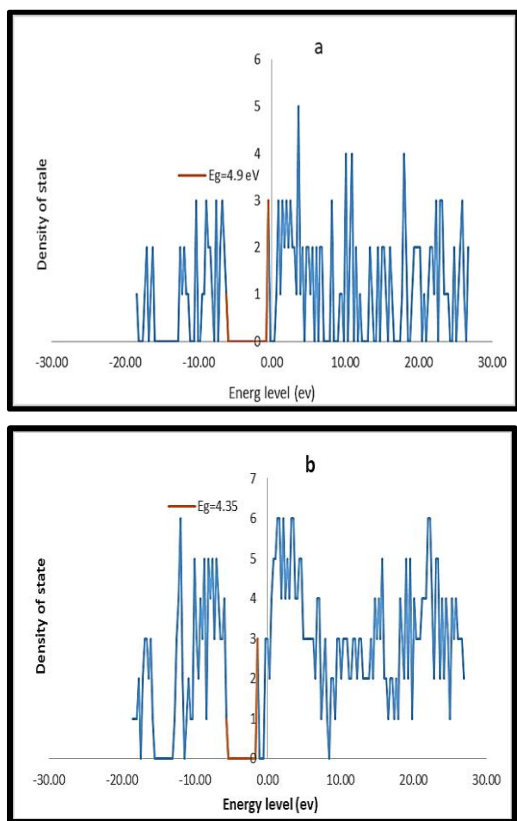


Figure (1): Density of State as a Function of Energy Levels using Base Group PBE/ 6-31G (d) for SiP-a-Diamamentan & b-SiP-Octamentan

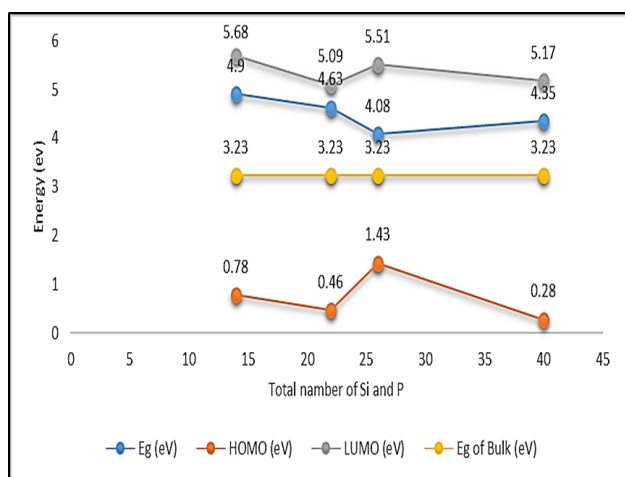


Figure (2) shows the energy gap and levels of HOMO, LUMO as a function of the total number of atoms of SiP, at the base group PBE/ 6-31G (d)

Figure (3) shows the longest and shortest bonds where the longest bond is at SiP and shortest at Si-H and p-H. Thus, the smallest value of the

bond is when both Si and P are connected to a single hydrogen atom with 1.91\AA which is the smallest value for Diamamentan that is an approximate to empirical value. While, the longest bond is when Si, P is linked to two hydrogen atoms with 1.90\AA value in Octamentan.

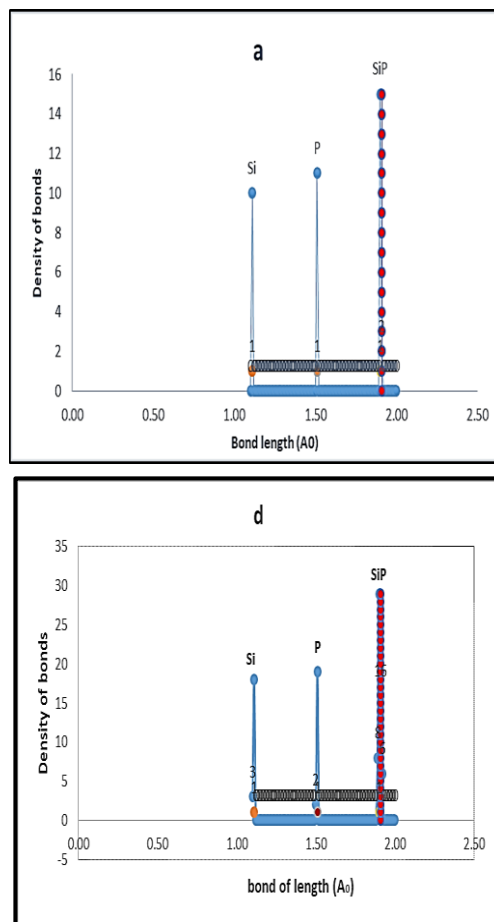


Figure (3): clarifies the density of the bonds as a function of the length of the bond in SiP-a-Diamamentan & b-Octamentan using the base groups PBE/6-31G (d) where the intermittent line represents the length of the experimental bond at 1.91\AA

All four tetrahedral angles have perfect values at 109.43° . Figure (4) shows the density of tetrahedral angles in SiP for Diamamentan and Tramamentan. The highest value for SiP for Diamamentan, is 110° ; while the highest value for SiP for Tramamentan is 109° . It is noted that the density of the tetrahedral angles of Tramamentan is much closer to the ideal values of 109.43° , which is due to the effect of surface



reconstruction which has a significant effect on all atoms.

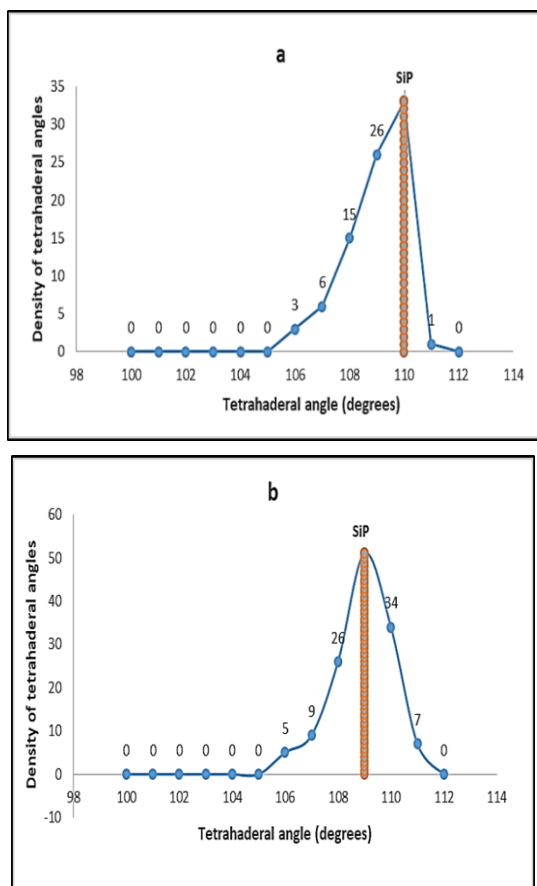


Figure (4) Density of tetrahedral angles for SiP for a–Diamamentan & b-Tramamentan. The intermittent line represents the ideal value for tetrahedral angles at 109°

The density of dihedral angles has one of the following values (180, -180, 60, -60). Figure (5) illustrates the values of the angles of Diamamentan and Octamentan that recorded at the values of 61, -61. But this is not quite true for the angles of SiP Octamentan. Therefore, the position should improve to be close to -58, 58 and be close to its ideal value.

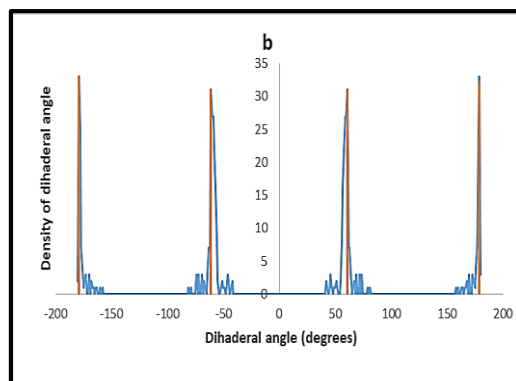
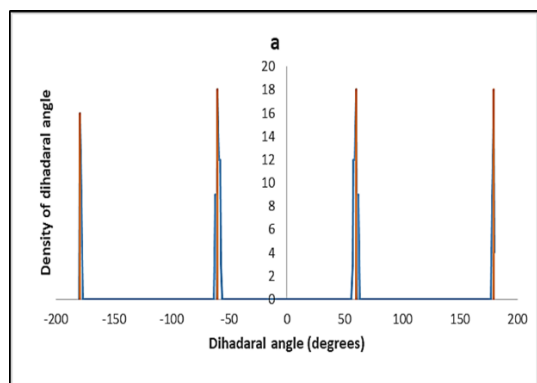
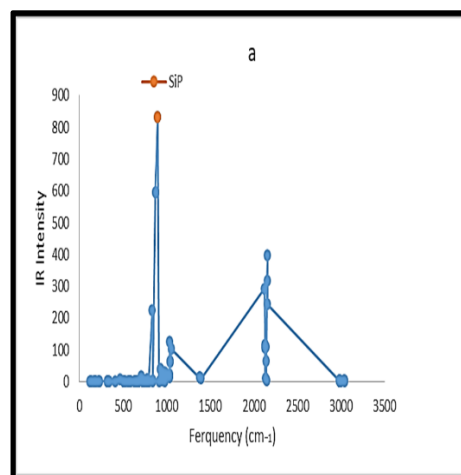


Figure (5) Density of dihedral angles in SiP for Diamamentan & Octamentan. Intermittent lines are at the ideal value for dihedral angles to SiP crystal (i.e. $\pm 60^\circ$ or $\pm 180^\circ$).

Figure (6) illustrates the IR spectrum of SiP structure molecules (Diamamentan & Octamentan) using the base group PBE/6-31G (d). Where the area can be divided into two parts based on the vibration properties or the gap between them, good results have been shown in the first area that starts from 0 to 300 cm⁻¹ and is an approximate to experimental results that have pure silicon. It is noted that the area around the wide peak at 657.11cm⁻¹, is a shift in frequency of about 100cm⁻¹ with increased frequency intensity infrared vibration due to an increase in the size of diamonds containing conditions 2000cm⁻¹-2400 in vibrations of Si-H, P-H



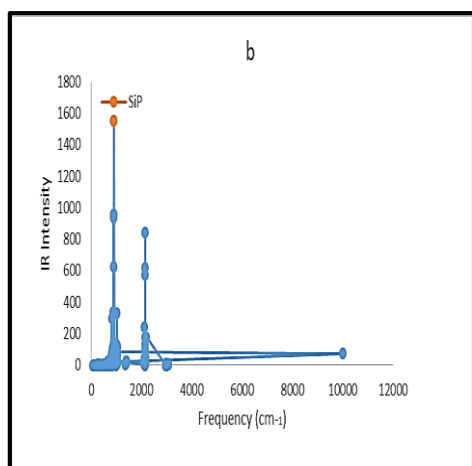


Figure (6) IR intensity as a function of the frequency intensity of SiP using base groups PBE/ 6-31G (d) for both a-Diamamentan & b-Octamentan

Conclusion

The properties of Sip nanocrystals and mass can be used with the corresponding molecular properties. As diamonds showed minimal surface relaxation effects that were inferred from their bonds' length, tetrahedral angles, dihedral angles, power gap and de-polarization. Consequently, the lengths of SiP bonds were found to be affected by the reconstruction of the surface. It is noted that the shortest Si-P bond between atoms, does not connected to surface hydrogen atoms. Furthermore, tetrahedral angles and dihedral angles showed an approximate with ideal values when larger diamonds were obtained. In addition to the density of energy state revealed the transition from individual energy levels to range structure along with the increase in diamond size.

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