

Abdullah Aufa Fuad, 2015. Kajian Ab Initio Molecular Dynamic Struktur dan Sifat Elektrik Gold Nanoparticle. Skripsi S1 fisika ini di bawah bimbingan Andi Hamim Zaidan, M.Si Ph.D dan Drs. Adri Supardi M.Si, Fakultas Sains dan Teknologi, Universitas Airlangga, Surabaya.

ABSTRAK

Tujuan dari penelitian ini adalah untuk mengetahui karakteristik struktur dan sifat elektrik *gold nanoparticle* (GNP) melalui kajian *ab initio molecular dynamic* (AIMD). Karakteristik struktur dibahas melalui analisa jumlah ikatan, distribusi sudut, dan fungsi distribusi radial. Sifat elektrik dibahas melalui analisa struktur pita dan rapat keadaan. Sampel GNP yang digunakan adalah likuid, amorf, dan icosahedral. Perhitungan dilakukan numerik menggunakan perangkat utamanya SIESTA. GNP likuid didominasi jumlah ikatan 9, GNP amorf 10, GNP icosahedral 18. Distribusi sudut ikat GNP likuid punya 1 puncak di 60° , GNP amorf punya 4 puncak di 60° , 90° , 120° , 175° , GNP icosahedral punya lengkap 6 puncak. Celah internal GNP likuid $2,7 \text{ \AA}$, amorf $2,8 \text{ \AA}$, icosahedral $1,9 \text{ \AA}$. Analisa struktur pita menunjukkan lebar celah pita GNP likuid $0,040 \text{ eV}$, amorf $0,071 \text{ eV}$, icosahedral $0,200 \text{ eV}$. Adapun lebar celah pita dari analisa rapat keadaan untuk GNP likuid adalah $0,053 \text{ eV}$, amorf $0,085 \text{ eV}$, icosahedral $0,200 \text{ eV}$.

Kata kunci: AIMD, SIESTA, GNP, jumlah ikatan, distribusi sudut, fungsi distribusi radial, struktur pita, rapat keadaan.

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ABSTRACT

The goal of this research is to know structural and electrical properties of gold nanoparticle (GNP) through ab initio molecular dynamic (AIMD) method. Structural properties are explained by the study of coordination number, bond angle distribution, and radial distribution function. Electrical properties are explained by the study of band structure and density of states. GNP samples used in this research are liquid, amorph, and icosahedral. The main software used for AIMD numerical calculation was SIESTA. Liquid GNP is dominated by coordination number of 9, amorph GNP 10, icosahedral GNP 18. Bond angle distribution of liquid GNP has 1 peak in 60° , amorph GNP has 4 peak in 60° , 90° , 120° , 175° , icosahedral GNP has complete all 6 peak. Internal spacing of liquid GNP is $2,7 \text{ \AA}$, amorph is $2,8 \text{ \AA}$, icosahedral is $1,9 \text{ \AA}$. Study of band structure show that the width of liquid GNP bandgap is $0,040 \text{ eV}$, amorph is $0,071 \text{ eV}$, icosahedral is $0,200 \text{ eV}$. While the width of bandgap by density of state study for liquid GNP is $0,053 \text{ eV}$, amorph is $0,085 \text{ eV}$, icosahedral is $0,200 \text{ eV}$.

Keyword: AIMD, SIESTA, GNP, coordination number, bond angle distribution, radial distribution function, band structure, density of state.