good accuracy. Hence, we have studied the D- and N-dependence of the HOMO-LUMO gap and optical gap along with N-dependence of the cohesive energy of tin quantum dots. It is observed that cohesive energy per heavy atom is increasing as far as the number of Sn atoms are increasing which is obvious. The HOMO-LUMO gap and optical gap, on the other hand, are decreasing with the increase in size and eventually obtain bulk crystal energy gap values. These properties are dominated by quantum confinement effect.

**Keywords:** Tin Nanoparticles; DFT calculations; Electronic properties; Structural properties; Cohesive properties

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## Effect of Silver Content on Thermal Properties of Ternary NiTiAg Alloys: Molecular Dynamics Simulation

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**Abstract:** Thermal properties of NiTiAg with different content of Silver investigated using Molecular dynamics (MD) simulation. Embedded atom method (EAM) potentials for describing of interatomic interaction are employed. However, the temperature and pressure of the system were controlled by Nose-Hoover thermostat and barostat. The melting of the ternary alloy was reflected through studying the temperature dependence of the cohesive energy and mean square displacement. To highlight the variances among ternary alloys with different content of Silver, the effect of Silver content on thermal properties containing the cohesive energy, melting point and isobaric heat capacity of fusion was estimated. It was revealed that the percent composition of silver are considerably affects the thermal properties. As a result, thermal properties of NiTiAg ternary alloy systems are higher than that of their corresponding of pure NiTi. However, Obtained results show that the melting point increases with decreasing of silver content of ternary alloys. It appears from MSD analysis that the diffusion coefficients of ternary NiTiAg alloys are directly proportional to silver content.

**Keywords:** Embedded atom method, Thermal properties, NiTiAg ternary alloy, means square displacement

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