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Order (n) tight binding molecular dynamics simulations of carbon nanotubes of various chiralities

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ABSTRACT

A Single Wall Carbon Nanotube (SWCNT) can be regarded as a rolled up graphene sheet with a diameter of about 0,7-10,0 nm. The orientation of six -membered carbon rings in the honeycomb lattice to the axis of the nanotube defines the structural and physical properties of SWCNT. With this orientation, CNT's have two main symmetry classification; achiral and chiral carbon nanotubes. Achiral carbon nanotubes have two classifications with the image of the hexagonal lattice through the axis of SWCNT. Zigzag and armchair CNT's. The structure of a SWCNT is specified by chiral vector (Ch=(n,m)), which corresponds to a section of the nanotube perpendicular to the nanotube axis (equator of the nanotube) [1]. The conductivity of SWCNT's is determined by chiral vector. A SWCNT can either be metallic or semiconducting depending on its diameter and chirality. Tight binding Molecular Dynamic (TBMD) is a useful method for studying the structural, dynamical, and electronic properties of covalent systems[2]. TBMD is computational tool designed to run finite temperature MD simulations within semi empirical tight binding scheme. This technique can be used to simulate material systems at different conditions of temperature, pressure, etc. including materials at extreme thermodynamical conditions. The traditional TB solves the schrodinger equation by direct matrix diagonalization and uses the simulation time in cubic scaling with the respect to the number of atoms ($O(N^3)$). On the other hand the Order N (O(N)) methods solve for the band energy in real space and make the approximations that only the local environment contributes to the bonding, and hence the band energy of each atom [3]. In this method, a large system is divided into many subsystems and its solution is found by summing solutions of each subsystems . In this case, the run time would be linear scaling with respect to the number of atoms . The O(N) TBMD technique has been applied to metallic (10,10) and semiconducting (17,0) carbon nanotubes successfully in [4],[5] and [6]. In this study, the same technique will be used in simulations of carbon nanotubes of various chiralities. First the O(N) algorithms will be explained. The necessary O(N) parameters will be fixed for each system. The canonical NVT molecular dynamics will be used to fix the temperatures of the carbon nanotubes. Physical properties and energetics of the various chirality carbon nanotubes will be reported.

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Metal basamaklı yüzeylerin titreşimsel özellikleri

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ABSTRACT

Bu çalışmada Yüksek Miller indisli (Düzenli basamaklı) Cu(551) yüzeyinin durum yoğunluklarının frekansa bağlı değişimi Real space Green's Function (RSGF) yötemi-(Gerçek uzay Green fonksiyonu) kullanılarak hesaplanmıştır. Bu yöntem için gerekli olan etkileşim matrisi Gömülü Atom yöntemi ile üretilen kuvvet sabitleri ile oluşturuldu. Yüzeydeki atomların yerel fonon durum yoğunlukları hesaplanarak, içte(Bulk) bulunan atoma karşılık gelen durum yoğunluğuna nazaran nasıl bir değişim gösterdiği incelenmiştir.Bu değişimin yerel atomik çevreye göre nasıl bir farklılık yarattığıda araştırılmıştır. Yüzey atomlarının yerel durum yoğunluklarında içteki atoma karşılık gelene nazaran düşük frekanslara doğru bir kayma gözlenmiştir.Ayrıca yerel atomik durum yoğunluklarının atomik çevreye duyarlı olduğuda gözlenmiştir. Atomik kuvvet sabitleri hesaplanarak atomik durum yoğunluklarında gözlenen bu temel özellikleri kuvvet alanlarındaki değişikliklerle ilişkilendirildi.

Generalized cluster variation theory for the isotropic-nematic phase transition

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ABSTRACT

In this study, a cluster variation theory depending on the Maier-Saupe model of the nematic-isotropic phase transition is generalized by using nonextensive formalism to examine the nematic-isotropic phase transition. This q-dependent formalism simplifies the cluster variation calculations compared with three- and four-particle cluster variation methods. The long range order parameter is investigated and the effect of the possible generalization is shown for some values of the entropic index q. Also the critical value of the long range order parameter at the nematic-isotropic transition temperature vs. the entropic index is reported.