VIBRATIONAL FREQUENCIES OF CLUSTERS: ARSENIC OXIDE, CARBON NITRIDE, COPPER OXIDE, SELENIUM AND RELATED COMPOUNDS WITH DIFFERENT ATOMS

AHMAD NAZRUL BIN ROSLI

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UNIVERSITY OF MALAYA
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Abstract

The density functional theory (DFT) has been used to solve the Schrödinger equation. The computer programmes have been developed which give a real advantage for solving large matrices in DFT that seem impossible to write by hand. The Amsterdam density functional (ADF) and DMol^3 of Accelerys have been used to calculate the vibrational frequencies of the atoms and molecules. The clusters of the molecules have been made for the study of glasses such as AgGeSe, AsSe, AsS, AsO, CuO, Se, FeP, FeAs, CN and graphene. These calculations are in good agreement with the experimental results. The local density approximation (LDA) and the generalized gradient approximation (GGA) both are used for solving eigen values of the Schrödinger equation. The double numerical and double numerical with polarized orbitals as a basis set for the wave functions are used in these calculations. The calculated frequencies have been compared with the experimentally measured Raman spectra to identify the clusters which are present in the material. This calculation is in accord with the experimentally observed Raman spectra.

Abstrak

Teori fungsi ketumpatan (DFT) telah digunakan dalam menyelesaikan persamaan Schrödinger. Program komputer telah dihasilkan dan memberi kelebihan kepada penyelidik untuk menyelesaikan matriks yang dahulunya mustahil untuk diselesaikan secara manual. Perisian Amsterdam density functional (ADF) dan juga DMol^3 dari Accelerys telah digunakan untuk mengira frekuensi getaran bagi atom dan molekul. Kluster bagi molekul-molekul kaca telah dibina seperti AgGeSe, AsSe, AsS, AsO, CuO, Se, FeP, FeAs, CN dan graphene. Keputusan dari pengiraan ini bersesuaian dengan hasil keputusan eksperimen. Penghampiran ketumpatan (LDA) dan penghampiran kecerunan umum (GGA) telah digunakan untuk menyelesaikan nilai eigen dalam persamaan Schrödinger. Numerik berganda (DN) dan numerik berganda beserta berkutub (DNP) digunakan dalam fungsi gelombang sebagai set asas untuk pengiraan ini. Frekuensi yang dikira telah dibandingkan dengan keputusan spektra Raman dari eksperimen untuk mengenal pasti kluster yang hadir dalam sesebuah bahan. Hasil pengiraan ini bertepatan dengan spektra Raman hasil dari eksperimen.

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