理论研究

二氧化硅准一维纳米团簇的弯曲振动

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摘要　运用密度泛函理论，计算了4～24个单元的准一维单链、双链、三元环、四元环管状构型SiO_2团簇的振动频率。在不同构型的红外光谱中，侧重研究了频率小于$300cm^{-1}$的低频处的弯曲振动。该类振动的频率和强度有很强的尺寸效应，频率与团簇长度呈指数关系，并且指数随直径变化表明它依赖于团簇的几何维数。实验发现此类红外振动只存在于长度0.8nm～5.5nm的SiO_2团簇中，揭示出实验和理论上可用于表征特定长度范围的纳米团簇。

关键词　准一维纳米团簇　红外光谱　尺寸效应　指数关系

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Bending mode of quasi-one-dimensional silica nano-clusters

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Abstract Vibration frequency modes of quasi-one-dimensional SiO_2 clusters with one chain, two chain, three- and four- membered ring structures were calculated according to the density-functional theory. The bending vibration at low frequency (less than $300cm^{-1}$) was emphatically investigated in the infrared spectrum with different conformation. This type of vibration mode shows strong size effect dependent on frequency and intensity, in which the frequency has exponential relations with the length of clusters. Furthermore, the variation of the exponent with diameter is corresponding to the geometry dimension of the clusters. It is found that such infrared vibration exists only at the length range of 0.8nm～5.5nm. The results reveal that the criterion can be used to characterize the specific length of nano-cluster in experiment and theory.

Key words quasi-one-dimension nano-cluster　infrared spectrum　size effect　exponent relation

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