Optical modes in nanoscale one-dimensional spin chains

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Abstract: The spin chain systems with one-dimensional magnetic ordering are promising candidates for quantum optical devices. This paper shows how the optical excitation can induce various phonon modes in an ideal Cu-O chain at various lengths. The calculation was carried out at different level theories including configuration interaction singles for excited states, density functional theory and second-order M??ller-Plesset perturbation. In general, the number of modes increases with chain length due to growing asymmetry of atomic positions when chain exceeds 5 nm. There were, however, only two basic modes: one is associated with the symmetric oscillation of oxygen and another with the asymmetric motion of the same along the chain. At the length below 4.3 nm, the Raman activity of the symmetric mode (440 cm^{-1}) dominates. From analysis of density of states, this mode may be associated with the excitation across the lowest LUMO bands with changing in spin state.

Author Keywords: Ab initio; Nanoscale; Optical phonon; Spin chain

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