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Gigahertz Oscillator of Carbon Nanotube: Molecular Dynamics Simulations

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This paper shows a possibility of gigahertz actuator composition based on multi-wall carbon nanotubes (CNT) encapsulating metallic ions using classical molecular dynamics simulations. Our results for a vacant CNT pendulum were in good agreement with results obtained from the previous experiments, theory, and simulations. Encapsulated potassium ions accelerated by applying external electric field could initialize the gigahertz actuator composed of a 7K*@CNT pendulum. The energetics and the operations of a vacant CNT pendulum were similar with those of the 7K*@CNT pendulum except for the binding energies, the correlated collisions, and the mass increase by the encapsulated ions. Since the total mass of the 7K*@CNT pendulum was slightly higher that of the vacant CNT one, the frequency of the vacant CNT one was slightly higher than the frequency of the 7K*@CNT one. The correlated collisions between ions or between the CNT and the ions slightly affected on the oscillation dynamics, such as restoring force and frequency.