Patterns of field electron emission from carbon nanotubes: Ab initio simulations by time-dependent density functional theory

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The experimental observation on carbon nanotubes (CNTs) using field emission microscope (FEM) clearly shows the symmetry properties of the CNT tips as well as the influence of adatoms [1]. Due to the localized states in nanostructures, it is desired to go beyond the traditional Fowler-Nordheim theory for clarifying the experimental FEM mechanism. Ab initio simulations are anticipated for this goal, however, previous studies based on density functional theory (DFT) calculations did not clearly show the relationship between the simulated current density distribution and the experimental FEM patterns, especially for the CNT-adatom systems [2].

In this study we present theoretical FEM patterns from pristine and H\textsubscript{2}-adsorbed CNTs, using ab initio time-dependent DFT [3]. The field-emitted electrons are treated in the equal footing with the electrons in the nanotubes, and the spatial distributions of current densities are calculated directly by the time-propagated Kohn-Sham wavefunctions. The simulated results of pristine CNTs clearly show either five-fold or six-fold symmetries, corresponding to the geometrical properties of pentagons in the CNT caps. Results of H\textsubscript{2}-adsorbed CNTs validate that the bright spots in the FEM pattern are attributed to the adsorption of the H\textsubscript{2} molecule. Our simulations demonstrate that the FEM patterns are largely contributed from the localized states in the tip of CNTs and there is a strong relation between theoretical and experimental results [4].