量子物理学・ナノサイエンス第 192 回セミナー

Controlling the optical properties of carbon nanotubes by chemical modification: computational studies

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日程　：　7 月 31 日（月）15:00–

場所　：　本館 2 階　H284B　物理学系輪講室

概　要

Single-walled carbon nanotubes (SWNTs) have characteristic luminescence peaks in near-infrared region. One of the main practical challenges of utilizing this luminescence is the low intensity of the peaks due to low-energy “dark” excitons. However, a radical increase of intensity as well as a red shift can be observed for nanotubes after chemical modification in their wall. We study the effect of such modifications, ozone doping and sp^3 doping of SWNTs, using Density-Functional Tight-Binding (DFTB) method. Dopants like ozone and several sp^3 dopants break the symmetry of the nanotube locally, allowing radiative transitions from the previously “dark” excitons. Some chemical modifications also create excess spin-density on the carbon nanotube wall, leading to preferential patterns of doping and controllable luminescence peaks. We also briefly discuss possible chemical strategies to control the optical properties by proximal doping. DFTB offers a significant speedup compared to DFT, which makes it especially suitable to study such local distortions and electronic states of systems at nano-scale.

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2017 年 7 月