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Optical Absorption Spectra of Charge Doped Single-Walled Carbon Nanotubes from First-principles Calculations GUANGFU LUO, Department of Physics, Peking University, JING LU, WAI-NING MEI, LU WANG, LIN LAI, JING ZHOU, RUI QIN, HONG LI, ZHENGXIANG GAO, DEPARTMENT OF PHYSICS, PEKING UNIVERSITY COLLABORATION, DEPARTMENT OF PHYSICS, UNIVERSITY OF NEBRASKA AT OMAHA COLLABORATION — The optical absorption spectrum of single-walled carbon nanotubes (SWCNTs) under charge doping is often interpreted within the graphene zone-folding and rigid-band model. Based on the periodic boundary model together with a uniform background countercharge, our density functional theory calculations, however, show that the spectrum response deviates from the expectations of such model. Specifically, the SWCNT band structures can differ qualitatively from the zone-folding ones, and with the increasing doping level, the absorption peaks will blench in a non-sequential energy order. The on-tube bands in SWCNTs sometimes change obviously even under low charge doping level, and accordingly cause spectra peaks to shift, split, and merge. At the end of this paper, we discuss briefly the applicability of the present results at the GW-BSE theory level and in other SWCNT-like systems.

Guangfu Luo
Department of Physics, University of Nebraska at Omaha

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