

Physikalisches Kolloquium

Thursday, 30.04.15, 17:15, HS 100
Reception with coffee & cookies 16:45

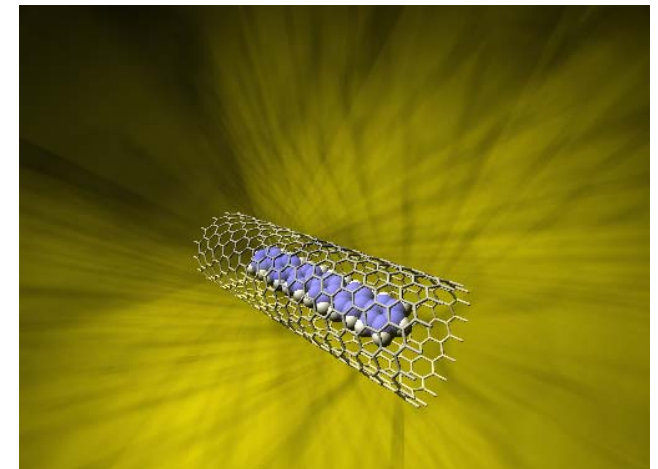


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Theoretical spectroscopy: Concepts and challenges for novel functional materials

Abstract

Ab initio spectroscopy is a powerful combination of quantum-based theories and computer simulations, covering a wide range of theoretical and computational methods which go beyond density-functional theory by incorporating many-body effects and interactions showing up in the excited state. This methodology not only allows for analyzing data obtained by experimental probes like photoemission, optical absorption, Raman, infrared, X-ray, and electron-loss spectroscopy, but also for shining light onto the underlying processes. Molecular materials – low-dimensional molecular arrangements as well as their interfaces with inorganic counterparts challenge these theoretical concepts. A series of selected examples will show where we are in our theoretical understanding, and what the major issues are that need to be tackled.



All of you interested in physics are cordially invited!