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Title: Into the origin of optical activity of carbon nanotubes

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Optical activity (OA) is the physical phenomenon associated to the rotation of linearly polarized light when it propagates through chiral compounds. Chirality is important in physics, chemistry, and biology, and plays a major role in biochemistry and pharmacology, and today it becomes an important issue in nanoscience. Nanoscale materials are used for asymmetric catalysis, analysis, separation, and also as molecular devices. Whether the goal is to use nanostructures for new approaches to solving problems in chiral technology or to use molecular chirality to engineering useful properties in nanoscale materials, this area is fruitful and exciting and certainty to continue to attract interest for the years to come. To understand chirality and other related effects, we recently developed a first-principles method to study the natural OA of nanostructures, making large-scale calculations of circular dichroism (CD) feasible. This methodology provides support for the quantification, understanding, and prediction of chirality and its measurement in nanostructures. In this talk, we present results for two different chiral nanostructures, which offer new kind of functionalized systems with novel properties. Our study is useful for the identification and quantification of chirality in these nanostructure, giving theoretical support to recent experiments. The system under study is carbon single-wall nanotubes (SWNTs), where tremendous progress has been made toward the synthesis of monodisperse samples. However, most of the SWNTs mixtures have a broad range of diameters, and chiralities, which are unsuitable for applications. Recently, scientists have turned their attention to sorting right- and left-handed SWNTs by wrapping they with chiral surfactants. The selection of a nanotube depends on the chiral agent and the specific helicity seems depend on which enantiomer is used. We discuss recent experiments in these systems.