Magneto-Optic Spectroscopy of Graphene Quantum Dots by First Principles

Jarkko Vähäkangas, Perttu Lantto and Juha Vaara

NMR Research Group, Department of Physics, Geosciences and Chemistry, P.O. Box 3000, University of Oulu, Finland
Jarkko.vahakangas@oulu.fi

In Faraday rotation, the plane of polarization of linearly polarized light beam rotates when it propagates through a material which is exposed to a magnetic field directed along the direction of propagation. Recently graphene has gained attention due to its capability to rotate the polarization plane by 6^{o}. Such high rotation power was earlier predicted to occur only in much thicker materials - not a single sheet of carbon layer [1].

More recently, in nanometer-size molecules that consist of finite arrangements of aromatic benzene rings, regarded as graphene quantum dots (GQDs), have been observed to feature collective electron oscillations called as molecular plasmons [2].

The Faraday rotation caused by the external magnetic field can be characterized with the Verdet-constant (V), whereas the nuclear spin optical rotation angle (NSOR) characterizes the rotation arising from the net magnetisation of nuclear spins [3]. Both parameters can be used to characterize molecules and belong to the family of magnetic optical spectroscopies. In this computational study those particular methods are for the first time utilized for different types and sizes GQDs to provide potential atomic resolution analysis tools for distinguishing them. In addition, it has been studied how point defects in GQDs influence the optical rotation properties.

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