APS March Meeting 2019

View Abstract

CONTROL ID: 3097211

TITLE: Orbital magneto-optical response of periodic insulators from first principles

Abstract Body: We present a reformulation of density matrix perturbation theory for time-dependent electromagnetic fields under periodic boundary conditions, which allows us to treat the orbital magneto-optical response of solids at the ab initio level. We use time-dependent density-functional theory (TDDFT) with the Sternheimer equation, implemented in the Octopus real-space code, to solve for the gauge-invariant part of the density matrix via the modern theory of polarization. Our computational scheme has an efficiency comparable to standard linear-response calculations of absorption spectra. Calculations of magnetic circular dichroism spectra for adenine, cyclopropane, and bulk silicon agree with the available experimental data. A clear signature of the valley Zeeman effect is revealed in the magneto-optical spectrum of a single layer of hexagonal boron nitride, with a g-factor similar to that observed in monolayer transition-metal dichalcogenides. The present formalism opens the path towards the study of magneto-optical effects in strongly driven low-dimensional systems.

PRESENTATION TYPE: Oral

UNIT: 16.0 GENERAL THEORY, COMPUTATIONAL PHYSICS (DCOMP)

SORTING CATEGORY: 16.01.04 First-principles modeling of excited-state phenomena in materials (DCOMP, DCP, DMP) [same as 05.01.07, 36.16.01.04]

Category Type: Computational

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