First Principles Simulations of the Optical Rotation in Oriented Systems with Periodic Density Functional Theory

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This contribution presents simulations of the optical rotation of chiral crystals using periodic density functional theory methods. The full Buckingham-Dunn tensor (see Fig. 1) is computed using a periodic formalism for the electric dipole, magnetic dipole, and electric quadrupole integrals.[1] The approach is used on a variety of test systems to investigate the effect of the choice of approximate functional, basis set, and gauge for the multipole operators.[2] The effect of intermolecular interactions is also investigated and compared to the intrinsic optical rotation of chiral molecular units.

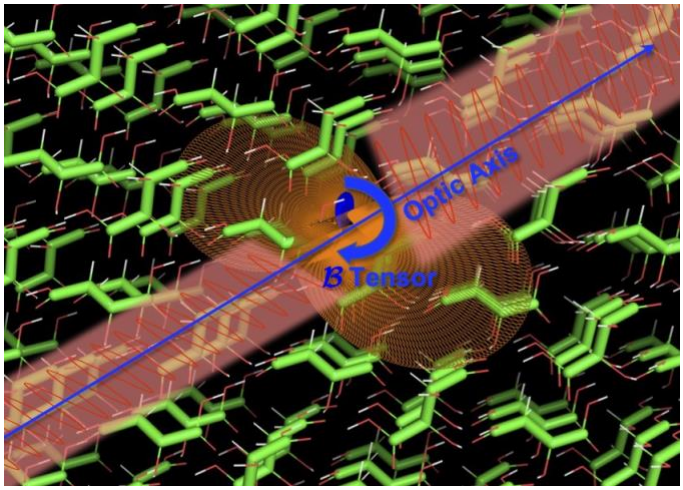

Figure 1. OR tensor for the (2R,3R)-tartaric acid crystal.

[1] T. Balduf and M. Caricato. "Derivation and implementation of the optical rotation tensor for chiral crystals". *J. Chem. Phys. 157* (2023), 214105. DOI: 10.1063/5.0130385.

[2] M. Caricato and T. Balduf. "Origin invariant full optical rotation tensor in the length dipole gauge without London atomic orbitals". ". *J. Chem. Phys. 155* (2021), 024118. DOI: 10.1063/5.0053450.