

Abstract Submitted
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Time-Dependent Molecular Response with both Electric and Magnetic Fields¹ RACHEL GLENN, ANDREW JAMES, T. DANIEL CRAWFORD, Virginia Tech — Time-dependent molecular simulations of optical spectroscopy conventionally consider the electric field strength much stronger than the magnetic strength. The various molecular dynamics contributing to a optical spectrum of a molecule in solution are time-dependent, some occur in the early time response (rotational-degrees) and some on a longer time response (translational-degrees) of the molecule. This has motivated us to develop time-dependent molecular response theory with both the magnetic and electric fields included. Here, I will discuss the our movement towards time-dependent quantum chemistry, and our recent results with the optical activity of chiral molecules.

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