Solvation, Coupled Cluster Response Theory, and the Optical Properties of Chiral Molecules

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The optical properties of chiral molecules are among the most challenging to predict, even for state-of-the-art quantum chemical methods because of their delicate dependence on a variety of intrinsic and extrinsic factors, including electron correlation, basis set, vibrational/temperature effects, etc.[1]-[4] This task is made even more difficult by solvation, which can have a dramatic impact on even the sign of optical rotation angles or circular dichroism rotational strengths.[5] In this lecture, we will discuss the most recent efforts from our group to attack this problem, including both implicit and explicit solvent models, and the role of reduced-scaling techniques to improve the efficiency of such computations.

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[2] T.D. Crawford, *Theor. Chem. Acc.* **115**, 227-245 (2006).

[3] M. Pecul and K. Ruud, *Adv. Quantum Chem.* **50**, 185-212 (2005).

[4] T.D. Crawford, M.C. Tam, and M.L. Abrams, *J. Phys. Chem. A* **111**, 12057-12068 (2007).

[5] J.M. Lambert, R.N. Compton, and T.D. Crawford, *J. Chem. Phys.* **136**, 114512 (2012).