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Determination of vibrational circular dichroism spectra of fluxional molecules through classical polarisable molecular dynamics

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Vibrational circular dichroism (VCD) is the weak difference in absorption for chiral molecules between right- and left- polarized light in the infrared range. It has promising applications in pharmacology owing to its ability to determine absolute configurations of chiral molecules. The shape of VCD spectra is highly sensitive to minor changes in conformation and molecular interactions, which makes it a sensitive probe of conformational isomerism and solvation [1].

As an alternative to methods based on explicit descriptions of electronic structure [2] and to circumvent their limited sampling capabilities in time and space, we have attempted to simulate the VCD spectrum directly from molecular dynamics trajectories employing a polarisable force field, extending earlier efforts dedicated to the IR spectrum [3]. In this presentation, we describe our implementation of VCD spectroscopy using the AMOEBA polarisable force field [4] in the Tinker software package [5]. We also report our first applications to solvated and solid amino acids, emphasizing the roles of temperature and the environment on the VCD spectrum. To determine the accuracy of the force field, we compare our results to those obtained with first principle molecular dynamics.

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