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Chirality transfer from chiral solutes and surfaces to achiral solvents: Insights from molecular dynamics studies

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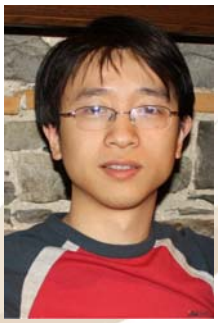
Chirality can be induced in achiral solvents located near a chiral molecule or surface. To capture the chirality transfer in solvent molecules, new polarizable and flexible models that are sensitive to the changes in the environment were developed based on an extensive series of *ab initio* calculations and molecular dynamics (MD) simulations. The models include electric field dependence in both the atomic charges and the intramolecular degrees of freedom. A multiple time step algorithm was implemented to deal with the simultaneous variation of the atomic charges and the intramolecular potentials. The methodology of developing these models is discussed in the first part of this presentation.

In the second part of this presentation, the chirality transfer from chiral solutes to achiral solvents is discussed. MD simulations of solvated chiral analytes formed the basis of the study. The chirality induced in solvents was assessed based on a series of related chirality indexes and the impact of conformational averaging was examined by comparing the chirality transfer about rigid and flexible solutes.

The chirality transfer from chiral surfaces to achiral solvents is also discussed. Emphasis is place on the extent of this chirality transfer and its dependence on the surface and solvent characteristics. Three surfaces that are commonly employed in chiral chromatography were examined. Since induced solvent chirality depends on the solvent position relative to the surface, a position dependent chirality index was analyzed in detail.



Shihao Wang obtained a B.Sc. in chemistry in 2004 from Nanjing University (China) and a Ph.D. in Computational Chemistry from Queen's University in 2009 under the supervision of Prof. Natalie M. Cann. His graduate researches focused on the development of polarizable models and molecular dynamics studies of chirality transfer. He is now a post-doctoral fellow with Prof. Guillaume Lamoureux at Concordia University, working on the computational studies of ammonium transport through membrane proteins and the parameterization and development of semi-empirical models.