

While working toward my Ph.D., I will perform research on **discontinuous molecular dynamics (DMD)** of **hydrogen bonding** and **polar** compounds. My goals will include developing methods for including effects of **dipole moments** in our methodology (**SPEAD**), adapting the methodology to prediction of **interfacial properties**, extending the methodology to broader ranges of compounds, improving the methodology for predicting **transport properties**, and improving the methodology for predicting **mixture phase equilibria**. We seek only mixing rules that reproduce our **molecular simulation** results. In other words, all **theory** and **simulation** must be entirely consistent with the dictates of the **intermolecular potential functions**. If there are errors in the intermolecular potentials at that stage, then we know where the problem is and we proceed to enhance the accuracy of the intermolecular potentials. It is a combination of **classical engineering thermodynamics** and **modern molecular simulation**. We are working on **transport** as well as **thermo** properties and we are interested in making the connection to **electrostatic potentials** and **mesoscopic systems**. Therefore, we should move in the direction of **field biased methods** for **mesoscale systems**. The idea of a **field-biased approach** is to use **DMD** for integrating the **repulsive motions** and biasing the **collision dynamics** in accordance with the force from the **Ewald summation**. We are also looking at ways of incorporating **quantum calculations** to estimate alterations in intermolecular potentials. Finally, we would like to implement the **DFT (Density Functional Theory)** methods of Tang and coworkers to account for the effects of attractive forces on fluid structure and to adapt the methodology to apply the reference structure from **DMD/TPT (Discontinuous Molecular Dynamics/Thermodynamics of Perturbation Theory)** simulation in combination with the **transferable force fields** developed for the **SPEAD (Step Potentials for Equilibria and Dynamics)** model. Hence, we need to demonstrate applications to **renormalization group scaling** in the **critical region** and **interfacial density profiles**. Tang and coworkers showed how RG (Renormalization Group) theory can be applied to the **DCF (Direct Correlation Function)** to correct the behavior in the critical region. Our question is whether the same approach can be adapted to the **SPEAD** characterization of molecules. If necessary, the **SPEAD** characterization could be in the form of a **SAFT (Statistical Associated Fluid theory)** representation for computing the correction in the critical region. I.e. we could identify an equivalent number of **tangent sphere segments** for each molecule and compute the RG correction by following Tang's method fairly closely. Elliott and Gray described how to make the connection to tangent sphere chains for n-alkanes. We would need to identify criteria for turning on the critical correction because we would expect it to be somewhat **expensive** computationally.