Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Effective Many-Body Interactions in Dipolar Fluids and their Effect on Structure: Can the Dipole-Dipole Interaction be Modelled as a Short-Ranged 3-Body Interaction? JULIEN SINDT, PHILIP CAMP, University of Edinburgh — In the 1970s, Stell *et al.* showed that it is possible to map the partition function of a system of particles interacting via anisotropic dipolar pairwise interactions to that of a hypothetical system with isotropic many-body interactions. It follows that "polar and nonpolar fluids have the same critical exponents" irrespective of long-ranged Coulombic interactions. We have calculated the structural properties of a system of soft spheres with the leading-order 2- and 3-body terms of the isotropic many-body potential. We have compared radial distribution functions and structure factors obtained from NVT Monte Carlo simulations with those from molecular dynamics simulations of dipolar soft spheres (DSSs) under the same physical conditions. We find that the many-body potential overemphasises chaining when compared to the equivalent DSS system. The chain-inducing component is the three-body Axilrod-Teller potential, and by adjusting its contribution, it is possible to match the structure with that of the DSS fluid, showing that the many-body potential can be used as a proxy for the dipolar potential. We conclude by studying the gas-liquid phase transition, finding that the phase transition disappears beyond a threshold degree of chaining.

Julien Sindt
University of Edinburgh

Date submitted: 13 Nov 2014 Electronic form version 1.4