

## A new formulation of the Isomorph Theory - and beyond

*Thursday, March 9, 2017 4:30 PM (45 minutes)*

The original formulation of the Isomorph Theory [1] predicts that some liquids have “isomorphs”, i.e., lines of invariant dynamics, structure and excess entropy in parts of their phase diagram. Here we present a new - and more elegant - version of the theory, which from a single assumption regarding the scaling properties of the high-dimensional potential energy surface predicts the existence of isomorphs [2]. Furthermore, the new version of the theory solves some of the (few) problems of the original version, e.g., the variance of heat capacity along an isomorph is now accurately predicted. Finally, we will discuss the extension to “pseudoisomorphs” in liquids with intramolecular vibrational degrees of freedom [3].

[1] N. Gnan, T.B. Schröder, U.R. Pedersen, N.P. Bailey, and J.C. Dyre, “Pressure-energy correlations in liquids. IV. ‘Isomorphs’ in liquid state diagrams”, *Journal of Chemical Physics* v131, p234504 (2009)

[2] T.B. Schröder and J.C. Dyre, “Simplicity of condensed matter at its core: Generic definition of a Roskilde-simple system”, *Journal of Chemical Physics*, v141, p204502 (2014).

[3] A.E. Olsen, J.C. Dyre, and T.B. Schröder, “Communication: Pseudoisomorphs in liquids with intramolecular degrees of freedom”, *Journal of Chemical Physics*, v145, p241103 (2016).

**Presenter:** SCHRØDER, Thomas (Dept. of Sciences, Roskilde University, Roskilde, Denmark)