# Ph.D. scholarships in the structure and dynamics of *Matter*

A number of Ph.D. scholarships are available linked to the Matter project beginning July 2017. Funded by the VILLUM Foundation and directed by Prof. Jeppe C. Dyre, Matter is an integrated part of the *Glass and Time* group (http://glass.ruc.dk) at Roskilde University's Department of Science and Environment. Over the coming years the project will employ seven Ph.D. students, six two-year postdocs, and three research professors.

The overall purpose of Matter is to determine the range of validity of the isomorph theory for the structure and dynamics of liquids and solids with "hidden scale invariance" (see, e.g., Dyre (2014) and Dyre (2016)).

One Ph.D. scholarship begins October 1, 2017, or soon thereafter, the next two January 1, 2018, or soon thereafter. We invite applications relating to one of the following six research topics.

NB: In the electronic application form's first entry "Description of the project" you merely state which of the six below research topics your application relates to and briefly give your qualifications for the particular research topic chosen; no detailed project description is required.

## Physical aging

*Background:* Physical aging is the gradual change of material properties due to adjustments of molecular positions. We have a unique experimental setup for monitoring such processes allowing for fast temperature changes (2 seconds) and extreme temperature stability ($\pm$100 μK). Last year we published two aging papers not using isomorph theory. One presented the first algorithm for calculating a non-linear relaxation curve directly from another (Hecksher *et al*, 2016), one identified theoretically the material time of the Narayanaswamy (1971) aging theory (Dyre, 2015).
*Scientific questions:*

- Does the Narayanaswamy theory hold only for R simple systems?
- How to develop a general framework describing the physical aging of R simple systems?

## Isomorph jumps

*Background:* An early prediction (Gnan *et al.*, 2009) was that following a jump between two thermodynamic state points on the same isomorph, the system is instantaneously in equilibrium because the Boltzmann statistical weights are the same for uniformly scaled configurations. As a consequence, jumps between two isomorphs should give identical relaxations, but in-house experiments by Professor Kristine Niss have revealed a more complex picture.
*Scientific questions:*

- How to develop a theory for jumps controlled via pressure, not density?
- How does this connect to the Narayanaswamy theory of physical aging?

**Coarse-graining**

*Background:* In a paper in preparation we show that even systems with weak virial potential-energy correlations may have isomorph-like curves - "pseudoisomorphs" - along which many, though not all, aspects of structure and dynamics are invariant (Olsen *et al.*, 2016). This shows that the isomorph theory applies even more widely than first anticipated.

*Scientific questions:*

- How to systematically identify a coarse-graining leading to pseudoisomorphs?
- Do all systems permit a coarse-graining resulting in lines of invariance for the structure and dynamics of certain degrees of freedom?

**Equations of state and quasiuniversality**

*Background:* The new theory of quasiuniversality (Dyre, 2016) relates to the condensed liquid phase, i.e., to liquid states that are not too far from the melting line - as well as to the entire crystalline phase. There are, however, intriguing recent suggestions of quasiuniversality also for the gas phase, even close to the critical point (Orea *et al.*, 2015).

*Scientific questions:*

- Can the isomorph theory be extended to include also the gas phase?
- Is there a quasiuniversal equation of state for R simple systems?

**1/d expansion**

*Background:* A few months ago it was shown by Maimbourg and Kurchan (2016) that for atomic systems the isomorph theory is exact in many dimensions. Assuming that this applies also for molecular systems one is led to the following conjecture: R simple systems are those that in three dimensions are "already" like their high-dimensional analogous, i.e., with dominance of first-coordination shell interactions (Ingebrigtsen *et al.*, 2012), whereas for complex systems the transition to simple behaviour takes place in more than three dimensions (Costigliola *et al.*, 2016) .

*Scientific question:*

- How to construct a systematic 1/d expansion going from the simple, high-dimensional limit to three dimensions?

**Quantum systems**

*Background:* The definition of an R simple system refers to a specific property of the potential-energy function. So far we have only studied systems obeying classical mechanics, which is generally believed to describe the motion of matter's atoms or molecules.

*Scientific questions:*

- Supposing a quantum system's potential-energy function obeys the R simple condition Eq. (2), which simplifications arise for its genuine quantum properties, e.g., Bose condensation?
- Is there a connection between the isomorph-theory quasiuniversality and that of Ho (2004)?

## References

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