

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* center (<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:

Physical aging [Experiments, possibly also simulations]

Background: Physical aging is the gradual change of material properties due to adjustments of molecular positions. *Glass and Time* has a unique experimental setup for monitoring such processes allowing for fast temperature changes (2 seconds) and extreme temperature stability ($\pm 100 \mu\text{K}$). Recently 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.*, 2015), 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, i.e., systems with isomorphs?
- How to develop a general framework describing the physical aging of R-simple systems?

Isomorph jumps [Experiments, possibly also simulations]

Background: An early isomorph-theory 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 and coworkers 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 [Simulations and theory]

Background: 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 [Simulations and theory]

Background: A new theory of quasiuniversality (Dyre, 2016) deals with the condensed liquid phase, i.e., liquids not far from the melting line - as well as with the entire crystalline phase. There are, however, intriguing recent suggestions of quasiuniversality also for the gas phase and 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 [Theory, possibly also simulations]

Background: Recently 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 for atomic systems going from the simple, high-dimensional limit to three dimensions?
- How to generalize the 1/d expansion to molecular systems?

Quantum systems [Theory, possibly also simulations]

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, which simplifications arise for its genuine quantum properties, e.g., Bose condensation?
- Is there a connection between the isomorph-theory of quasiuniversality and that of Ho (2004)?

References

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Ho T.-L. (2004), Phys. Rev. Lett. **92**, 090402.
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We are looking for ambitious and open-minded persons with a master's degree in physics or a related field. The successful applicant has also strong mathematics skills and enjoys the close interaction between theory, simulation, and experiment that is emphasized in the *Glass and Time* center.

For further information you are welcome to contact Prof. Dyre at dyre@ruc.dk .

Employment is regulated by an agreement between the Ministry of Finance and the Central Organization of the Academics; thus Ph.D. students have the same rights, formal working hours, vacation, etc., as others in the workforce. After taxes the monthly salary is approximately 16000 DKK (2100 Euro).

Roskilde University welcomes applications from candidates of any social and ethnic backgrounds irrespective of gender, age, religion or any other irrelevant criteria.

Application is submitted via Roskilde University's website <https://ruc.dk/en/phd-scholarships-roskilde-university> . Deadline: September 1, 2017.