

PCoMS: Seminar Series on Multiscale Theory for Materials [1]



Date: February 19 (Wed.), 2020 10:30~12:20

Venue: A4-115 Katsura Campus,
Kyoto University (Kyoto)

Title: Soft-matter materials modeling in the data-driven era

Speaker: Prof. Dr. Tristan Bereau

Van't Hoff Institute for Molecular Sciences and Informatics Institute,
University of Amsterdam
Amsterdam 1098 XH, The Netherlands
t.bereau@uva.nl

Advanced statistical methods are rapidly impregnating many scientific fields, offering new perspectives on long-standing problems. In materials science, data-driven methods are already bearing fruit in various disciplines, such as hard condensed matter or inorganic chemistry, while comparatively little has happened in soft matter.

I will describe how we use multiscale simulations to leverage data-driven methods in soft matter. We aim at establishing structure-property relationships for complex thermodynamic processes across the chemical space of small molecules. Akin to screening experiments, we devise a high-throughput coarse-grained simulation framework. Coarse-graining is an appealing screening strategy for two main reasons: it significantly reduces the size of chemical space and it can suggest a low-dimensional representation of the structure-property relationship.

To illustrate these aspects, I will model the passive translocation of small molecules across a phospholipid bilayer. Our systematic exploration generates predictions for more than 1 million small molecules, and connects key functional groups to the thermodynamic process. I will further outline recent results on the screening of small molecules to drive phase transitions in lipid mixtures.

For the details and further information, please contact
PCoMS office [pcoms\[-at-\]imr.tohoku.ac.jp](mailto:pcoms[-at-]imr.tohoku.ac.jp) (Please change [-at-] with @.)

*PCoMS: Professional development Consortium for Computational Materials Scientists
<http://pcoms.imr.tohoku.ac.jp/>

**Post-K Exploratory Challenge, Sub-Challenge B: Phase Transitions and Flows
<https://www.cbsm2.imr.tohoku.ac.jp/>