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Multiscale modeling of organic materials

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Propositions

accompanying the dissertation

Multiscale Modeling of Organic Materials

From the Morphology Up

by

Riccardo Alessandri

1. The combination of solvent evaporation simulations and a modular coarse-grain force field, such as Martini, is currently the best solution to simulate the morphology of organic materials. [Chapter 2 and 3 of this thesis]
2. The functionalization of organic molecules with polar side chains increases the energetic disorder in their solid state films. [Chapter 4 of this thesis]
3. The building block approach underlying the Martini model, providing the model its ease of use, comes at a price if not considered carefully. [Chapter 5 of this thesis]
4. A wealth of questions exist that can be answered by applying Martini (3) in soft materials science. [This thesis]
5. When choosing a methodology for your investigation, besides the timescales of the processes which need to be simulated, consider also the timescale of interest for the problem.
6. A false intellectual appearance is counterproductive. It does not enable knowledge sharing nor is it useful for building sympathy.
7. Collaboration can be one of the most engaging, and fruitful endeavours in science.
8. One of the hardest things to do these days is to embrace boredom.