Modelling the nucleation of proteins into amyloid fibrils

Stefan Auer, University of Leeds, UK

Fibrils of amyloid proteins are currently of great interest because of their involvement in various amyloid-related diseases and nanotechnological products. In my talk I will present my attempt to model amyloid fibril nucleation. The use of a coarse-grained protein model enabled me to calculate a peptide phase diagram [1] and to investigate the importance of kinetics in protein aggregation [2]. Because such simulations are computationally very time consuming, we also used a lattice model to quantitatively predict nucleation rates [3]. It turns out that the obtained supersaturation dependence of the rate could not be described adequately by nucleation theories, which demanded a new theoretical treatment that we presented recently [4].

[1] S. Auer and D. Kashchiev, Phys. Rev. Lett. 104, 168105 (2010)
[2] P. Ricchiuto, A. Brukhno, S.Auer, J.Phys.Chem.B, 116, 5384 (2012)
[3] R. Cabriolu, D. Kashchiev and S. Auer, J. Chem. Phys. 137, 204903 (2012)
[4] D. Kashchiev, R. Cabriolu, S. Auer, J. Am. Chem. Soc. 135, 1531 (2013)

Thursday, December 12th, 2013
16:00 (Room 1.079)

Institute for Computational Physics, Allmandring 3