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S E M I N A R
aus
Halbleiterphysik und Nanotechnologie

Di, 3.7.2018, 11:00 Uhr, Hörsaal für Physik

"Stochastic models of disordered mesoporous materials for small-angle scattering and more"

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Small-angle scattering of x-rays (SAXS) or neutrons (SANS) is one of the few experimental techniques that can be used to investigate porous materials *in situ* over length scales from 1 to 100 nm. The experimental potential of the method, however, is often hindered by the lack of data analysis procedures to convert scattering data into structurally meaningful information. This is the case for many porous materials of practical interest, which are inherently disordered. In that context, the main difficulty consists of finding a balance between (i) the realism of the model that should capture the geometrical complexity of the material, and (ii) its conceptual simplicity that is required for the robustness of the analysis as well as for its practicality. Stochastic methods offer a way through these almost antagonistic requirements [1].

The seminar will present in a non-technical way a few stochastic models useful for small-angle scattering analysis of disordered mesoporous materials. The various models - Boolean, dead-leave, and Gaussian field models - differ notably by the connectivity and tortuosity of the material's pores and solid phase. We will also discuss how the stochastic approach is extended to model not only the porous material but also phases confined in the pores. These extended models can be used for analysing *in-situ* scattering data [2], as well as for developing physicochemical models of confined phenomena that account for the complex structure of the host material [3].

[1] C.J. Gommes, Stochastic models of disordered mesoporous materials for small-angle scattering and more, *Microp. Mesop. Mater*., 257 (**2018**) 62-78;
[2] C.J. Gommes, Three-dimensional reconstruction of liquid phases inside disordered mesopores using in-situ small-angle scattering, *J. Appl. Crystallogr*. 46 (**2013**) 493-504;
[3] C.J. Gommes & A.P. Roberts, Stochastic analysis of capillary condensation in disordered mesopores, *Phys. Chem. Chem. Phys*. (**2018**) DOI: 10.1039/C8CP01628C.