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26. Oktober 2012

Einladung zum Vortrag

von

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UNIVERSITÄT ULM, INSTITUT FÜR STOCHASTIK

Stochastic modeling of the 3D morphology of energy materials on various length scales

The morphological 3D structure of complex porous or composite materials is closely related to their physical properties, in particular with transport processes of charges, gases, or fluids, and with degradation mechanisms occurring in these materials. Thus, the systematic development of 'designed' 3D morphologies with improved physical properties is an important problem which has various applications, e.g., in Li-ion batteries, organic solar cells, and fuel cells. Mathematical models from stochastic geometry can help to solve this problem, since they can be used to provide a parametric description of complex 3D morphologies in existing materials. Moreover, systematic modifications of model parameters and the combination of stochastic morphology models with numerical transport models offer the opportunity to construct new 'virtual' (but still realistic) 3D morphologies with improved physical properties, using model-based computer simulations.

In this talk we present several types of models from stochastic geometry which have been developed for complex 3D morphologies of energy materials on various length scales. First, we discuss two different stochastic modeling approaches for the 3D microscale structure of electrodes in Li-ion batteries: a germ-grain model for the pore phase of uncompressed electrodes, and a graph-based model for the solid phase of compressed electrodes. In both cases the models are fitted to experimental 3D data gained by synchrotron tomography. Then, we consider a germ-grain model for mesoscale morphologies of photoactive layers in organic solar cells which have been fitted to 3D image data from electron tomography. It turns out that the quality of percolation pathways, considering the charge carrier mobility, and also the exciton quenching efficiency strongly depend on the mesoscale morphology. Finally, we discuss a 3D network model on a molecular scale for charge transport simulations in large domains of amorphous organic semiconductors and we show how the usage of segmentation methods can reduce computational costs of such simulations by several orders of magnitude.

Termin: Samstag, 10. November 2012, 10:30 Uhr
Ort: Hauptgebäude der Universität Ulm, Raum 252

Der Vortrag findet im Rahmen des Workshops „Stochastik in der Praxis" anlässlich des Wima-Kongresses statt. Interessenten sind sehr herzlich eingeladen.

gez. V. Schmidt