

## Kolloquium für Mechanik

Referee: **Dr. Xiaoying Zhuang**  
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Date: Thursday, April 18, 2019, 15:45h  
Location: Bldg. 10.81, HS 62 (R 153)

Title: **Multiscale Methods and Probabilistic Optimization for Computational Materials Design of Nanocomposites**

### Abstract

The development of novel man-made materials is among the main reasons that made transistors and computers much faster, many electronic devices smaller and cheaper or medical implants more compatible. The key criteria for the choice of a material w.r.t a specific application are the macroscopic properties, such as fracture toughness, electromechanical and thermal properties. However, the macroscopic properties are governed by the features and interactions at a much finer length scales. For the design of a new material, it is therefore of utmost importance to understand and quantify the effects taking place at the finer scale and how they are linked to the coarser scales.

In this talk, Dr. Zhuang will present her recent works for the characterization, optimization and design of new nanocomposites and nanostructures. Special focus will be given on novel computational methods for addressing challenging issues including: 1) bridging the length/time scales and the transfer of the model information between the discrete nanoscale (atomistic) to the continuum-scale; 2) Optimization and inverse design with targeted functions accounting for the uncertainties propagation through different scales. Finally, the talk will be concluded by highlighting the perspectives of using machine learning for integrated material engineering such as for finding new metamaterial and design of topological insulator.

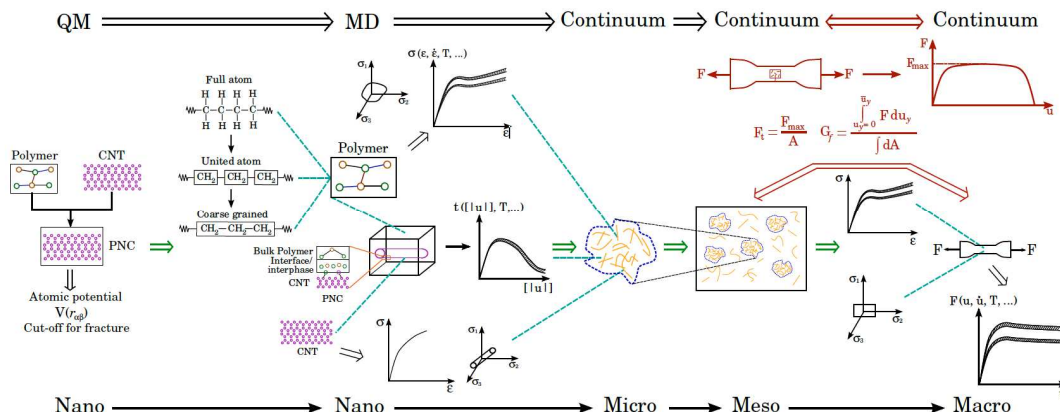


Figure: Framework of multiscale model for polymeric composite material

References:

- [1] Uncertainties propagation in metamodel based probabilistic optimization of CNT/polymer composite structure using stochastic multi-scale modeling. Computational Materials Science, 85: 295-305 2014.
- [2] Topology optimization of flexoelectric nanostructures. Journal of the Mechanics & Physics of Solids, 105:217-234, 2017.
- [3] Intrinsic bending flexoelectric constants in two-dimensional materials, Physical Review B, 99:054105, 2019.

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Alle Interessenten sind herzlich eingeladen.  
Prof. Dr.-Ing. Thomas Böhlke