

**Research Network: Multiscale Simulation of Solids**

**Research Project: Multiscale Modeling of Advanced Materials with Microstructure**

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### **Summary**

Complex macro-phenomena in solid materials such as nonlinear hystereses, developing anisotropies, size effects, phase transitions and multi-field coupling effects require new modelling techniques, which directly take into account mechanisms occurring at the microstructure. The key perspective towards a reliable description of these effects is provided by multiscale approaches which reduce the empiricism of purely macroscopic theories by accounting for the evolution of microstructure with model-inherent scale bridging techniques. The rootage of these techniques in recently developed variational-based homogenization and relaxation methods for dissipative systems provides a promising methodology towards the design of a new generation of predictive material models and their efficient numerical implementation. Based on the experience of the research group on homogenization- and relaxation-based computational scale-bridging techniques for composites, polycrystals, polymers and granular materials, the project intends to investigate a new class of complexity in the multiscale modeling of solids. On the one side, this will cover the development of new variational-based homogenization methods for (a) extended continuum formulations of materials accounting for non-local size-effects and multifield phenomena. On the other side, we will underline these developments by new variational-based (b) discrete-continuum bridging techniques between molecular dynamics, lattice statics, discrete dislocation dynamics and the above mentioned continuum formulations. The research on advanced materials focusses on crystalline solids with regard to the macroscopically predictive simulation of inelastic size-effects and fracture as well as thermo-, electro- and magneto-mechanical bulk-hysteresis phenomena. From the viewpoint of the methodology, the project provides a basis for the design of new functional materials by generating virtual test environments with direct access to micromechanical properties.