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PROGRAMMVORSCHAU

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"Exploring nanomaterials with multiscale simulations for interface and interphase engineering"

Johannes Kepler Universität Linz
17.15 Uhr, HS 12 (TNF-Turm)

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Exploring nanomaterials with multiscale simulations for interface and interphase engineering

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Abstract
Current developments and coarse-Graining schemes aimed to achieve models retaining molecular specificity will be described. To this aim, models combining particle and continuum representations are proposed. In particular, descriptions based on combination of molecular models and field theory [1] or molecular models and finite elements methods (FEM) [2] will be described. Hybrid models, due to their computational efficiency, are gaining popularity (for recent reviews [3-5]). This framework allows to develop coarse-grained models with high chemical specificity suitable for industrial applications but at the same time, using an efficient parallelization scheme,[6] opens the possibility to simulate large-scale systems. Current developments and several applications of MD-SCF technique, ranging from self-assembled structures[7] to polymer melts [8], to rational design of polymer composites[9] and a microscopic description of macroscopic properties [2,10] will be described.

Keywords: Polymer Composites, Gas Sensors, Biopolymers, Molecular Simulations

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