Contribution ID: **598** Type: **Oral (Non-Student) / orale (non-étudiant)**

Multiscale modeling of multifunctional, hybrid and nanomaterials: from quantum chemical and microscopic to coarse-grained level with an effective pair potential

Thursday, June 18, 2015 4:45 PM (15 minutes)

The steady increase in the complexity of new industrial materials and the need to accurately predict their properties have resulted in rapid development of sophisticated methods of modelling on multiple length and time scales. A simple hierarchical approach combines different methods for different scales (quantum mechanical, microscopic, mesoscopic) interpreted independently. Information obtained at one level is transmitted to the next level without critical assessment or performance improvement. An advanced hierarchical approach works in a similar manner but with a feedback control. In these approaches, continuous (macro- and mesoscale) properties of materials stem from and can be controlled with their microscopic structure. To connect to large scales, molecular models representing microscopic structure must be coarse-grained to reduce detailed degrees of freedom while preserving relevant ones. The industrial importance of coarse-graining techniques to connect multiple length and time scales and to properly take into account the most notable mesoscale phenomena is increasingly appreciated. When implemented in software packages, such modelling techniques significantly accelerate development of new materials satisfying modern industrial requirements. In this contribution, we present and discuss a hierarchical procedure of bridging the gap between atomistic and macroscopic modelling through mesoscopic level of description. Its successful application is demonstrated on examples of multi-scale modelling and synthesis of polyester ionomers, to explain gelation mechanism and prefigure gelation ability of oligomeric electrolyte gelators, and to predict both structural and dynamic properties of polymer solutions with high accuracy and computational efficiency. To this end, we develop a new methodology which replaces the heuristically defined interaction potential in dissipative particle dynamics (DPD) with an effective pair potential obtained using molecular theory of solvation, and validate the method on a well-studied real system. The methodology is free from artificial restrictions on potential range and shape and also eliminates solvent from DPD, which enormously increases computational efficiency.

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Session Classification: R3-2 Polymers and Biopolymers (DCMMP-DMBP) / Polymères et biopolymères (DPMCM-DPMB)

Track Classification: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)