



Use of Multi-Scale Simulation for Material Innovation

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Message from the Guest Editor

We are living in a material world, designing functional material is key. In absence of validated data for materials, one therefore need to perform high throughput simulation to generate good property data to run data modeling to innovate new material in today's world of informatics. Molecular modeling based on molecular structure can be used to predict key properties to gain insight into the behavior of the materials and calculate properties that are relevant to material engineers. Macro scale simulation is in place to look into device properties, where the material properties comes from some standard database (there are very few databases with mixed material properties) as input and if unavailable it still is a guess, and with a vast new materials in practice; this is becoming a challenging task. Multi-scale simulation is therefore is an effort to link the gap between microscale to macro-scale through meso-scale. In this time with a new demand for new materials is the time to have the special issue to improve our understanding on this.





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