

Challenges and opportunities in modeling functional nanostructured materials for future technologies

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In this talk, I will illustrate how we can model functional nanostructured materials for future technologies in sustainable chemistry, nanosensing, and clean energy. Our society faces challenges like providing clean, affordable energy, protecting natural resources, combating pollution, and mitigating climate change. Functional nanomaterials are crucial for developing technological solutions to these issues. Experimentally, it is very difficult to link nanometer scale structural modifications to the macroscopic function. Modelling these materials in close synergy with experiments can provide nanoscopic insights and lead to design of materials for future technologies.

Nanostructured materials used in applications are far from perfect, with heterogeneities in space and time across various scales. These spatial heterogeneities, from subnanometer to micrometer, affect the material's dynamics. The functional behaviour is also influenced by operating conditions. There is a significant gap between theoretical and experimental length-time scales. This talk will overview the current state of modeling functional nanostructured materials and the challenges in mimicking experimental conditions. The concepts will be illustrated through applications in sustainable chemistry, clean energy, and nanosensing.