

## **Computationally understanding and designing functional materials for energy applications: From nanoscale to realistic mesoscale models**

*Sven M.J. Rogge, Veronique Van Speybroeck*

Computational research provides necessary insight to characterize, understand and design functional nanostructured materials. However, the increasing complexity of these high-end materials, as well as the stringent design criteria they need to meet, pose fundamental challenges for experimental and computational researchers alike. In this presentation, recent advances in computational material research at the Van Speybroeck group at the Center for Molecular Modeling will be highlighted through four case studies, performed in close collaboration with different experimental partners. In a first case study, we'll investigate how strain engineering helps to achieve stable and efficient all-inorganic perovskite solar cells at room temperature. From a computational perspective, this requires both highly accurate electronic structure methods and structural models that achieve the necessary length scales over which these strain fields arise. Second, we'll focus on how computational simulations help to understand the formation and stabilization of clathrate hydrates in hydrophobic mesoporous materials, which can in turn be used for hydrogen transport. A third case study will highlight our recent understanding of how zeolitic imidazolate frameworks can be used as efficient and reusable nanofluidic shock absorbers for high-rate impacts. Herein, we'll focus on the myriad of complementary computational tools necessary to model the spatiotemporal behaviour of these materials, given the large variety of length and time scales that play a role during shock absorption. Finally, we'll briefly introduce our approach to design covalent-organic frameworks for Z-scheme photocatalytic applications.

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