Special Issue

Modeling Adsorption Properties of Molecular and Nanostructured Systems for Environmental Applications

Message from the Guest Editors

Understanding how adsorption properties towards common pollutants can be improved offers the possibility of solving emerging ecological problems. In terms of aspects of renewable energy, it is also imperative to find materials with superior adsorption properties towards molecular hydrogen. Various molecular and nanostructured systems have been proposed for the efficient adsorption of pollutants and hydrogen, but the quest for perfect adsorbing materials remains open. Ab initio and density functional theory (DFT) calculations, molecular dynamics (MD) simulations and other approaches are indispensable computational tools in the area of adsorption research. A perfect adsorbing material should allow both adsorption and desorption under mild conditions to allow further technical processing of adsorbed molecules, while the adsorber can be recycled several times. This imposes several research challenges, such as appropriate interval of binding energies, specific adsorption mechanisms, high adsorbing capacity, etc.

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