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Hindawi

Special Issue on

Computational Modeling of Adsorption Properties of Molecular and Nanostructured Systems for Environmental Application

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Understanding how adsorption properties towards common pollutants can be improved offers the possibility to solve emerging ecological problems. From the renewable energy aspects, it is also imperative to find materials with superior adsorption properties towards molecular hydrogen. Various molecular and nanostructured systems have been proposed for efficient adsorption of pollutants and hydrogen, but the quest for perfect adsorbing materials remains open. Density functional theory (DFT) calculations and molecular dynamics (MD) simulations 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 mechanism, and high adsorbing capacity.

We would gladly consider computational studies dealing with adsorption properties of other systems, within the frame of proposal. The following are some potential structures for the computational studies of adsorption properties from the environmental.

Potential topics include but are not limited to the following:

- Nanotubes
- Fullerenes
- Buckybowls
- 2D structures
- Ionic liquids
- Metal oxide catalysts (TiO_2, ZnO, etc.)
- Sensor properties for polluting molecules
- Self-assembled monolayers

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Manuscript Due
Friday, 25 August 2017

First Round of Reviews
Friday, 17 November 2017

Publication Date
Friday, 12 January 2018