Designing Nanoporous Materials for Hydrogen Storage

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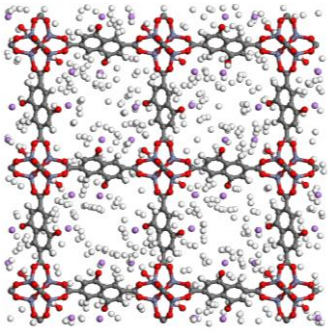
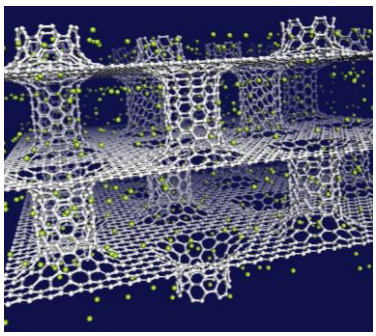
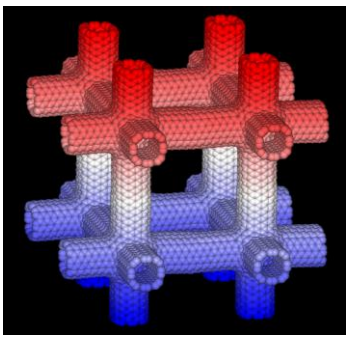
ABSTRACT:
A combination of *ab-initio* and Monte Carlo techniques is used for both, evaluating the hydrogen storage capacity of different materials 'in silico', and designing novel materials with enhanced storage capacity. Accurate *ab-initio* methods employed for investigating the nature of hydrogen interaction with different types of nanoporous materials, while Grand Canonical Monte Carlo simulations show their storage performance under different thermodynamic conditions. Carbon based materials and Metal Organic Frameworks (MOFs) are intensively investigated in different scales of size and theory. The storage capacity of Nanotubes (C-NT, BN-NT, SiC-NT) [1-3], Nanoscrolls [4], MOFs [5] and COFs is evaluated under various conditions of temperature and pressure. Novel materials like *pillared graphene* [6] were designed and tested. Finally, the improvement of the storage capacity by functionalization [7] and doping [8] is evaluated under various thermodynamic conditions.

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