Gas storage and separation using three-dimensional pillared graphene oxide frameworks with phenyldiboronic acid linkers: A computational approach.

Ioannis Skarmoutsos$^{1,2}$
Emmanuel N. Koukaras$^1$, Emmanuel Klontzas$^2$
$^1$Aristotle University of Thessaloniki, Department of Chemistry, 54124, Thessaloniki, Greece
$^2$National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, Vas. Constantinou 48, 11635, Athens, Greece
Contact@iskarmou@eie.gr

Abstract

Potential applications of previously synthesized three-dimensional pillared frameworks of graphene oxide layers interconnected with phenyldiboronic acid linkers [1,2] in the field of gas storage and separation have been systematically explored using a combination of density functional theory calculations and Grand Canonical Monte Carlo simulations. A systematic computational screening of the efficiency of such frameworks in the capture and separation of a wide variety of potent greenhouse gases, as well as gases with significant applications in the energy sector, such as hydrogen and natural gas constituents, has been performed. An effective classical interaction potential model was employed for the pillared graphene oxide frameworks, using the intramolecular geometry and charge distribution from the quantum chemical calculations performed in the present treatment and adopting well-established Lennard-Jones parameters for the nanoporous material and existing accurate potential models for the molecular gases under investigation. The results obtained have revealed that this particular class of porous frameworks can have significant applications in industrial processes related to gas storage and separation, as well as in the capture of greenhouse gases to prevent global warming and climate change.

Acknowledgements: The authors acknowledge the funding from the Hellenic Foundation for Research and Innovation (HFRI) and the General Secretariat for Research and Technology (GSRT), under grant agreement no. 1536.

References