University of Crete
Department of Physics

Physics Colloquium

Thursday, 28 March 2019 | 17:00 – 18:00, Seminar Room, 3rd floor

Designing novel Nanoporous Materials for applications in Energy, Environment and Health: From Multi-Scale Modeling to Materials Informatics

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ABSTRACT

A combination of ab-initio, Monte Carlo and Molecular Dynamics techniques is used for designing novel nanoporous materials for various applications. Hydrogen, methane and CO_2 storage, natural gas processing, drug delivery and flexible electronics are some of the tasks that will be addressed and their connection to nanoporous materials will be analyzed.

Different type of strategically designed novel nanoporous materials like: Nanotube and Molecular Pillared Graphene [1], Porous Nanotube Networks [2], Super Diamond, Metal and Covalent Organic Frameworks [3-4], will be presented and their structural and electronic properties will be discussed. In addition, the root for the improvement of materials' properties with molecular engineering will be also demonstrated [5].

Finally, a novel computational methodology for large-scale screening of materials with the use of Machine Learning algorithms (ML) will be introduced [6].

References

[1] "Pillared Graphene: A New 3-D Network Nanostructure for Enhanced Hydrogen Storage" Dimitrakakis, G. K.; Tylianakis, E.; Froudakis, G. E. ***Nano Letters*** *8 (2008) 3166-3170.*

[2] "Porous nanotube network: a novel 3-D nanostructured material with enhanced hydrogen storage capacity" E. Tylianakis, G. Dimitrakakis, S. Melchor, J.A. Dobado and G.E. Froudakis, ***Chem. Commun****., 47(2011) 2303-2305.*

[3] "Designing 3-D COFs with enhanced hydrogen storage capacity." E. Klontzas, E. Tylianakis, G.E. Froudakis, ***Nano Letters****, 10 (2010) 452–454.*

[4] "Improving Hydrogen Storage Capacity of MOF by Functionalization of the Organic Linker with Lithium Atoms." Klontzas, E.; Mavrandonakis, A.; Tylianakis, E.; Froudakis, G. E. ***Nano Letters*** *8 (2008) 1572-1576.*

[5] "Enhancement of hydrogen adsorption in Metal-Organic Frameworks by the incorporation of the sulfonate group. A multiscale computational study", A. Mavrandonakis, E. Klontzas, E. Tylianakis, G.E Froudakis, ***J. Am. Chem. Soc****., 131 (2009) 13410–13414.*

[6] "Chemically intuited, large-scale screening of MOFs by machine learning techniques", Borboudakis, G; Steriannakos, T; Frysali, M; Klontzas, E.; Tsamardinos, I; Froudakis, G.E.;, ***Nature Computational Materials*** *3: 40 (2017).*

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