Novel 3D SiC and BN pillared nanostructures: design principles, electronic and H_2 storage properties.

T. Stergiannakos*, E. Klontzas, G.E. Froudakis
Department of Chemistry, University of Crete, P.O. Box 2208, 71003, Heraklion, Crete, Greece

E. Tylianakis
Department of Materials Science and Technology, University of Crete, P.O. Box 2208, 71003Heraklion, Crete, Greece

T. Vegge
Department of Energy Conversion and Storage, Technical University of Denmark, Frederiksborgvej 399 Building 238, DK-4000 Roskilde, Denmark

Novel three dimensional Silicon Carbide (SIC) and Boron Nitride (BN) nano-structured materials have been designed, based on Pillared Graphene (PG) architecture [1]. These novel materials, similar to PG, combine graphene-like sheets and nanotubes to form periodic 3D SiC and BN structures. The general Euler's rule for polygons was used to create the junctions that connect the 2D sheets with the nanotubes, by choosing proper combinations of different polygons (three octagons, six heptagons …). These novel materials present by design interesting features such as versatile geometric characteristics, tunable pore sizes and surface areas. Their structural and electronic properties were investigated by performing DFT calculations, while their Hydrogen adsorption properties were investigated by following a multi-scale theoretical strategy. Our results indicate that SIC-PG and BN-PG act as semiconductors and have better H_2 adsorption properties than carbon PG. This enhancement is attributed to the increased electrostatic nature of H_2 interactions with the consisting atoms of these materials [2][3]. Further enhancement of the H_2 storage characteristics was achieved by doping these materials with metal atoms.

References

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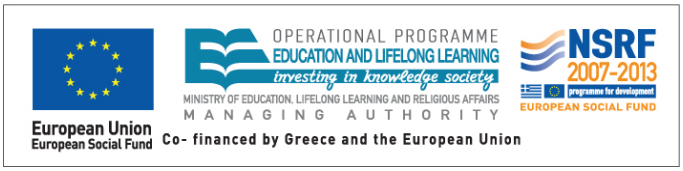

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* sterg_t@chemistry.uoc.gr