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NH-16, Anakapalle, Visakhapatnam-531002, Andhra Pradesh.

(IOTDA-2K21)

17-18 Dec, 2021

Department of Computer Science & Engineering
and Electronics & Communication Engineering

Proceedings of Two Day Online National Conference on Internet of Things : Design & Applications

Sponsored by

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Content

Predicting the Hydrogen Storage Capacity of Lithium Doped MWCNTs Nanoparticles using Machine Learning Techniques

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Abstract: Hydrogen storage is a key enabling technology as hydrogen is considered both a future automotive fuel and a medium for energy storage; however, its application has been limited by hydrogen's low volumetric density at ambient conditions. Current hydrogen-vehicle designs require storage systems based on high-pressure compression, which are costly and could pose safety issues. Design of novel storage systems that can deliver hydrogen with high energy densities have been a recent focus of many studies. In this context, computational approaches enabling fast and accurate predictions for the amount of stored hydrogen can play an instrumental role in the identification of outstanding materials on the computer, prior to laboratory synthesis and testing. In this issue MWCNTs are used to identify top-performing structures for hydrogen storage. Importantly, this study assesses the performance of 14 ML algorithms that correlate textural properties with their hydrogen storage capacities. These ML models were restricted to only seven structural features: single crystal density, pore volume, gravimetric surface area, volumetric surface area, void fraction, largest cavity diameter, and pore limiting diameter. Hydrogen adsorption was set for two operating conditions: i.e. 253 K and 298 K up to 70 bar pressure. Lithium decorated MWCNTs prepared in water; amine and DMF adsorb 0.81, 0.93 and 1.67 wt % of hydrogen at 253 K and 0.57, 0.87 and 1.31 wt % at 298 K respectively, at non-cryogenic temperatures and moderate pressures. Capacities are predicted for two operating conditions:

a.Usable gravimetric capacity in weight percent (Wt%), defined as the mass of stored H2 divided by the summed mass of H2 and the MWCNTs.

b.Usable volumetric capacity in grams of H2 stored per liter.

Keywords: Functionalization, P-MWCNTs, f-MWCNTs, Hydrogen storage