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Evaluation of Hydrogen Particle Volume on Surfaces of Selected Nanocarbons

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Abstract : This paper describes an approach to the adsorption phenomena modeling aimed at specifying the adsorption mechanisms on localized or nonlocalized adsorbent sites, when applied to the nanocarbons. The concept comes from the fundamental thermodynamic description of adsorption equilibrium and is based on numerical calculations of the hydrogen adsorbed particles volume on the surface of selected nanocarbons: single-walled nanotube and nanocone. This approach enables to obtain information on adsorption mechanism and then as a consequence to take appropriate mathematical adsorption model, thus allowing for a more reliable identification of the material porous structure. Theoretical basis of the approach is discussed and newly derived results of the numerical calculations are presented for the selected nanocarbons.

Keywords : adsorption, mathematical modeling, nanocarbons, numerical analysis
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