

Evaluation of adsorption properties of graphene

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Graphene as one of the carbon allotropes prepared in 2004 [1] is of great interests owing to its electronic and structural properties.

At the same time graphene can be powerful adsorbent with uniform very large specific surface area 2630 m²/g [2]. At present there are no methods of preparation of graphene in large quantities for the investigation of adsorption properties of graphene sheets. Although it is possible to produce large quantities of graphene by reduction of graphene oxides but graphene prepared by such method has chemical and physical defects.

Adsorption properties of graphene can be evaluated from numerous data on investigation adsorption properties of graphitized carbon black with uniform surface by chromatographic methods e.g. [3].

In [4] the potential energy functions for interactions between a carbon atom and monolayer graphite sheet, between a carbon atom and a semi-infinite graphite crystal were computed. From this data it is possible to assume that energy interaction of molecules with monolayer graphite sheet is about 90% of energy interaction with a semi-infinite graphite crystal. So from the data on adsorption properties of graphite (graphitized carbon black) it is possible to evaluate the heats of adsorption and adsorption equilibrium constant (Henry constant) of different organic compounds at small coverage on graphene sheets.

The contributions of different functional groups to the heats of adsorption and Henry constants were evaluated from the calculated data on heats of adsorption at small coverage and retention volumes (adsorption equilibrium constant) of organic compounds with different functional groups on graphene.

It is possible to calculate the thermodynamic characteristics of adsorption for great numbers of organic compounds on graphene by using these contributions.

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