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Ab initio study of the water adsorption on hydroxylated graphite clusters modelling soot surfaces.

B. Collignon (1) , P.N.M. Hoang (1), S. Picaud (1), and J.C. Rayez (2)

(1) Laboratoire de Physique Moléculaire, UMR 6624, Université de Franche-Comté, 16 route de Gray, F-25030 Besançon Cedex (France); (2) Laboratoire de Physico-Chimie Moléculaire, UMR 5803, Université de Bordeaux I, 351 cours de la libération, F-33405 Talence Cedex (France). (barbara.collignon@lpm.univ-fcomte.fr)

In this work, we study the interaction between small water aggregates and hydroxylated graphite surfaces by means of quantum calculations. The hydroxylated graphite surfaces are modelled by anchoring OH groups on the face side or on the edges of a graphite crystallite of nanometer size. The quantum calculations based on the ONIOM approach aim at characterizing the adsorption properties (structure and adsorption energy) of small water aggregates containing up to 4 water molecules, in order to better understand at a molecular level the role of such OH sites on the hydrophylic properties of graphite surfaces modelling soot emitted by aircraft.

The results of our calculations show that the OH group act as a nucleation center for small water aggregates containing up to 3-4 molecules, with mean adsorption energies per water molecule that range between -16.7 and -30.4 kJ/mol above the face, and between -19.3 and -33.1 kJ/mol above the edge of the hydroxylated graphite cluster.

These results have been compared with those obtained when considering adsorption of water above a COOH group anchored on the graphite surface, and show that a OH group appears less attractive than a COOH group with respect to water adsorption. Our results also indicate that such OH and COOH groups are rapidly saturated when increasing the water coverage, and a quite large distribution of such active sites is certainly necessary for a graphite surface to become hydrophilic