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Molecular modeling study on the water-electrode surface interaction in hydrovoltaic energy

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The global energy problem caused by the decrease in fossil fuel sources, which have negative effects on human health and the environment, has made it necessary to research alternative energy sources. Renewable energy sources are more advantageous than fossil fuels because they are unlimited in quantity, do not cause great harm to the environment, are safe, and create economic value by reducing foreign dependency because they are obtained from natural resources. With nanotechnology, which enables the development of different technologies to meet energy needs, low-cost and environmentally friendly systems with high energy conversion efficiency are developed. Renewable energy production studies have focused on the development of hydrovoltaic technologies, in which electrical energy is produced by making use of the evaporation of natural water, which is the most abundant in the world. By using nanomaterials such as graphene, carbon nanoparticles, carbon nanotubes, and conductive polymers, hydrovoltaic technology provides systems with high energy conversion performance and low cost, which can directly convert the thermal energy resulting from the evaporation of water into electrical energy. The effect of the presence of water on the generation of energy via the interactions between the ion(s) and the liquid–solid surface can be enlightened by the mechanism of the hydovoltaic effect. Here, we simply try to get some tricky information underlying the hydrovoltaic effect by using DFT/B3LYP/6-311G(d, p) computations. Namely, the physicochemical and electronic properties of the graphene surface with a water molecule were investigated, and how/how much these quantities (or parameters) changed in case of the water molecule contained an equal number of charges were analyzed. In these computations, an excess of both positive charge and negative charge, and also a neutral environment was considered by using the Na^+, Cl^-, and NaCl salt, respectively.

Natural water is the most abundant clean and sustainable resource on earth, covering approximately 71% of the earth's surface and capturing approximately 70% of the solar energy received by the earth's surface[1]. The excess energy in the water, which can flow and evaporate spontaneously by adsorbing thermal energy without being affected by environmental conditions, is separated from the surface in the form of latent heat[2,3]. The evaporation potential and current, which continues as long as the evaporation of water continues, provide the conversion of thermal energy into electrical energy[2,4]. Due to the unique characteristics of both the water molecule and graphene surface in terms of the structural, electronic, and thermal properties, water-graphene systems have been increasingly studied in many areas[5–7]. The graphene structure consists of the sp^2 hybridized carbon atoms and thus the electron delocalization on the surface plane is responsible for the in-plane heat conductivity, while out-of-plane thermal conductivity can be provided by the weak dispersion forces or van der Waals interactions[8]. Also, the water molecule has been reported with a vital role in the harvesting of new-generation energy such as kinetic energy by hydrovoltaic tools, gradient, and evaporation energy[9].

Hydrovoltaic systems, which produce electricity from the direct interaction of water with the material, are preferred instead of existing technologies used to obtain electrical energy from the kinetic energy of water. Energy from water is converted into electrical energy by hydrovoltaic effects provided by mechanisms such as flow potential, fluctuation potential, shrinkage potential and evaporation-induced electricity, and gradient-induced ion diffusion. When solids come into contact with water, ions with opposite charges to the surface charge are attracted and an electrical double layer (EDL) is formed at the water–solid interface. EDL-based electrokinetic effects, such as flow potential, can convert the kinetic energy of water flowing through narrow channels into

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