Density functional theory calculations on magnetic properties of FePc on Si(111)4×1-In surface

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Metal-organic systems have attracted much attention for potential applications in future electronic devices. Among these systems, metal phthalocyanine (MPc) represents one of the most promising classes because of its thermal and chemical stability. In recent years, there has been a variety of work performed on MPc systems such as FePc, CoPc, NiPc, and CuPc on graphene/Ni(111) [1-2] as well as on metallic surface [3-5]. However, it is scarcely known about them on nanostructured metal-semiconductor hybrid substrates. Theoretical analysis is highly required to understand issues such as the MPc-substrate interaction, which may affect the molecular adsorption mechanism and the magnetic properties on the metal/semiconductor hybrid surfaces. In this presentation, we report density functional theory (DFT) calculations on the FePc on Si(111)In-4×1. The results include a variety of adsorption sites and magnetic moment depending on sites which separate into In-chain, Si-chian, and boundary area. We found that the magnetic moment on the Si-chain area was the larger than on the In-chain area. The stable adsorption sites and electronic structure will be discussed.

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