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Fluorine-Induced Local Magnetic Moment in Graphene: A hybrid DFT study

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Recent experimental evidence that fluorinated graphene creates local magnetic moments around F adatoms has not been supported by semilocal density-functional theory (DFT) calculations where the adsorption of an F adatom induces no magnetic moment in graphene. Here, we show that such an incorrect prediction of the nonmagnetic ground state is due to the self-interaction error inherent in semilocal exchange-correlation functionals. The present hybrid DFT calculation for an F adatom on graphene predicts not only a spin-polarized ground state with a spin moment of $\sim 1\ \mu_B$, but also a long-range spin polarization caused by the bipartite nature of the graphene lattice as well as the induced spin polarization of the graphene states. The results provide support for the experimental observations of local magnetic moments in fluorinated graphene.

Keywords: graphene, magnetism, self-interaction error, DFT, hybrid functional, fluorinated graphene

S-002

PEDOT: PSS 박막의 대면적 나노패터닝을 통한 구조형성방법 및 응용

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오늘날 유기고분자기반 태양전지는 다른 태양전지와 비교될정도로 낮은 광변환효율로 인해 효율향상을 위한 많은 연구들이 진행되어 왔다. 그중 패터닝을 통한 광포집률과 charge carrier 수집효율이 증가되었다는 많은 보고들이 있었다. 따라서 우리는 200~1,400 nm polystyrene bead를 합성하여 air-liquid interfacial 방법을 이용해 2차원 육방조밀구조를 갖는 template를 형성하고 Nanosphere lithography (NSL)를 이용하여 대면적으로 균일한 poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS)를 패턴화하였다. 균일한 패턴형성을 측정하기위해 Field Emission Scanning Electron Microscopy (FE-SEM), image를 얻었으며, Atomic Force Microscopy (AFM)를 통해 형성된 패턴의 낙차 높이를 얻었고, Near IR-UV-Vis을 통해 bead size 변화에따라 얻어진 PEDOT:PSS 패턴의 반사율을 측정하였다.

Keywords: Organic photovoltaics, nanosphere, lithography, surface morphology, patterning