

2D carbon-metal frameworks for photochemical reactions promotion

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A wide range of 2D carbon allotropes have been predicted and theoretically explored during the last years [1–5]. It is noteworthy that in recent works there were proposed synthesis methods for production of the allotropes [6], which opens broad prospects for building nanostructures based on them, for example, different metal-carbon frameworks. Such systems exhibit interesting properties due to the presence of metal-carbon bonds like surprisingly stable metallocene molecules [7,8] which consist of metal atoms sandwiched between two cyclopentadienyl anions. In metallocene-like 2D nanostructures the metal atoms are protected by carbon sheets, while the metal atoms are placed in the middle of penta-rings of carbon atoms.

In our work we carried out a theoretical investigation of two 2D metallocene analogs based on graphene allotropes. The first system is a defected graphene monolayer functionalized by metallocene fragments. The second system is a novel 2D nanostructure consisted of two carbon layers and metal atoms (Co or Fe) sandwiched between them, which structure can be represented as metallocene molecules without hydrogen atoms organized into a 2D hybrid structure. By using density functional theory, we examined the stability of proposed structures and studied the features of electronic, magnetic, and optical properties. The Fe-filled structures exhibit semiconducting properties while Co-containing structures show half-metallic properties. Both demonstrate increased absorption spectra in the visible area, which together with changing oxidation degree make them excellent candidates for photoinduced catalytic reactions under sun irradiation. The work was supported by the Russian Science Foundation (№21-73-20183).

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