Endohedral complexes based on small fullerenes with metals as a basis for the formation of heterostructures

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Low-dimensional heterostructures find their application in electronics and optoelectronics: heterolasers, photodiodes, phototransistors, etc. have been developed on their basis. An extensive list of low-dimensional carbon materials, including graphene, carbon nanotubes, fullerenes, can be used as a basis for their production. Two-dimensional heterostructures are layered structures, the material of each layer of which differs from the others in the value of energy gap. We propose to consider small fullerenes C20, C24, C28 as a basis for the formation of such objects.

It is known that the presence of a cavity in fullerenes allows intercalating them with atoms and even small molecules. In our case we will consider endohedral complexes of fullerenes with metals: alkali (Li, Na, K) and transition (Ti, Zn). The introduction of metal atoms can significantly influence the properties of the systems, unlike, for example, atoms and molecules of inert gases, the introduction of which into the cavity of fullerenes often insignificantly affects their properties.

The study was carried out by quantum-chemical modelling methods in the framework of density functional theory in the B3LYP variant using the 6-311++G(d,p) and cc-pvDZ basis sets.

We have obtained optimised structures of endohedral fullerenes M@C20,24,28 (M=Li, Na, K) as well as Zn@C28 and Ti@C28, and calculated the values of the energy gap. Based on this, it was concluded that it is possible to form a heterostructures based on a number of these materials.

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