Nanocomposites and nanomaterials

Structure and Thermal Stability of Co- and Fe-Intercalated Double Silicene Layers

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By employing the methods of MM+, PM3 and Monte-Carlo, there has been studied the positioning of Co- and Fe-atoms in double silicene layers depending on their concentration and temperature, analogically [1]. The molecules have been found out to form stable interection metal atoms with silicene layers, and a tendency between intercalate stability the silicene structure. The temperature growth (over ~500 K for Co and over ~600 K for Fe) causes gradual bond ruining followed by extrusion of interlayers intercalate. Further temperature increase up to 600 K for Co and 700 K for Fe respectively is characterised with intercalate interlayers desorption (Fig. 1). There have been calculated the double silicene layers UV-VIS depending on intercalate concentration and the association constant of the system which makes 111.3 $l \cdot mole^{-1}$ for Co- and 71.1 $l \cdot mole^{-1}$ for Fe-system.

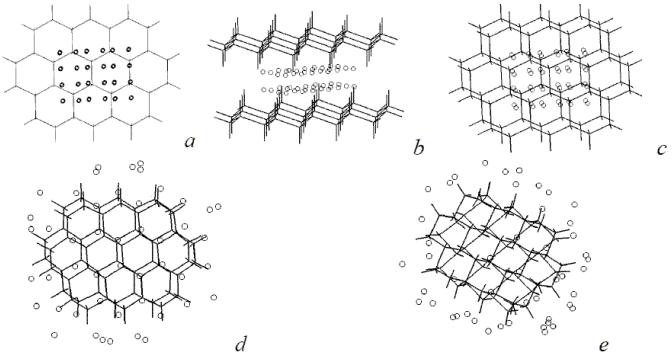

Fig. 1. Studied systems: *a, b, c* – the original structures projections; *d, e* – screenshot of configurational change of systems.

1. *Mykhailenko O.V., Prylutskyy Yu.I., Matsui D at all.* Structure and Thermal Stability of Co- and Fe-Intercalated Double Graphene Layers // J. Comput. Theor. Nanosci. – 2013. – Vol. 7. – N 6. – P. 996-999.