

## Theoretical Study of Metal Composite on the Monolayer PPAN Basis, Containing Pair Metal Atoms Cu-Co and Cu-Ni

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**Abstract** - In this work PPAN monolayer containing pair of atoms of metals Cu-Co, Cu-Ni is considered. The structure of the metal complex system was investigated. Single-electron spectra were constructed; the width of the energy gap was analyzed and compared with the similar characteristic of PPAN, which does not contain metal atoms. Binding energy is calculated and metal charges are carried out. Influence of copper atom on basic characteristics of metal complex is determined. The studies were performed using the DFT method with B3LYP functionality and cc-pvdz basis.

**Keywords:** Metallocarbon nanocomposite, Carbon-containing matrix, Pyrolyzed polyacrylonitrile, Paired metal atoms, DFT.