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Interaction between Functionalized Graphene with Ti/C and Histidine/Leucine: Effects of Charging

© *H.H. Gürel, B. Salmankurt*

Technology Faculty, Information System Engineering Department, Kocaeli University, Umuttepe Campus, 41001, Kocaeli, Turkey

E-mail: h.hakan.gurel@gmail.com

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In this work, theoretical calculations are modeled by using density functional theory including van der Waals effects. We have investigated the binding mechanism, as well as magnetic and electronic properties of basic amino acids such as histidine and leucine with titanium/carbon functionalized graphene. We also focused on the effects of charging on the structural, magnetic, and electronic properties. We have shown that binding energy and magnetic and electronic properties may be altered by adding or removing an electron to/from the system. Charging can change the band structure dramatically, so in some spin up/down cases, the system becomes semiconductor. Functionalization performing with charging allows us to design some spintronic devices and/or biosensors for detecting histidine and leucine for low concentration levels.

Keywords: graphene, charging, amino acids, histidine, leucine, binding.