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Electronic and transport properties of heme-b adsorbed on graphene nanoribbons EDUARDO CRUZ-SILVA, ORNL, MARCIA BOJORQUEZ-AVITIA, LINAN-IPICyT, RODOLFO CRUZ-SILVA, CIICAp-UAEM, FLORENTINO LOPEZ-URIAS, LINAN-IPICyT, VINCENT MEUNIER, ORNL, MAURICIO TERRONES, LINAN-IPICyT, BOBBY G. SUMPTER, ORNL
— Heme-B is the prosthetic group of several hemoproteins, such as several peroxidases and hemoglobin. It contains an Iron atom that can be oxidized or reduced depending on its environment. Changes in Iron oxidation state enable diverse biological functions like oxygen transport and electron transfer. In this work, we present a quantum density functional study on the adsorption of a heme-b group in graphene. The effects of heme-b adsorption on the graphene electronic structure will be shown. These changes have clear effects on the quantum transport properties of graphene, which coupled with the affinity of heme-b group to molecules like oxygen, carbon dioxide and carbon monoxide, could help to develop new graphene based amperometric biosensors.

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