

Surface Dimer Model in the Theory of Adsorption on Graphene

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Received: January 17, 2022

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Abstract. Model of the surface dimer formed by coupling adsorbing atom and surface substrate atom by covalent bond is proposed. This model is used for the calculations of the charge transfers between dimer’s atoms and between dimer and graphene substrate. Effects of Coulomb and electron-phonon interaction on charge transfers are thoroughly studied. Role of inter-adatoms dipole-dipole repulsion and exchange interactions are examined. Adsorption on epitaxial graphene is briefly discussed.

Acknowledgements. The work was supported by the Ministry of Science and Higher Education of the Russian Federation (Project 075-15-2021-1349).

Citation: Rev. Adv. Mater. Technol., 2022, vol. 4, no. 1, pp. 21–27

View online: <https://doi.org/10.17586/2687-0568-2022-4-1-21-27>

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