

Abstract Submitted  
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**A simple model for electronic properties of surface adsorbed molecules.** RAJESH DHAKAL, WILLIAM SCHWALM, University of North Dakota — We adapt a minimal approximation to one electron quantum theory of molecules referred to as Fast Accurate-Kinetic Energy method by F. Harris et al. to a Green function formalism. This in principle handles large complex molecular structures with less computational effort to compute electronic properties of adsorbed molecules. Kinetic energy integrals are calculated accurately but multi-electron potential energy integrals are approximated. The neighboring atom interactions are included also. The calculations are iterated to achieve a rough charge self-consistency. The method is expected to obtain qualitative suggestions of spectral features that can appear in experiments, thus relating such features conceptually to the physics of adsorbate systems. In the work presented, we study properties of graphene with adsorbate systems including isolated hydrogen atoms and vacancies in graphene lattice.

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