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A simple model for electronic properties of surface adsorbed molecules. RAJESH DHAKAL, WILLIAM SCHWALM, Univ of North Dakota — We adapt a minimal approximation to one electron quantum theory of molecules referred as Fast Accurate Kinetic Energy method. 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. For layers of isopthalic acids formed on pyrolytic graphite the configuration changes as a function of length of hydrocarbon tails. We study properties of this system as a function of tail length.

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