

Abstract Submitted  
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**The range of two-body adsorbate-adsorbate interactions on the surface of graphene** DMITRY SOLENOV, National Research Council, National Academies, Washington, District of Columbia 20001, CHAD JUNKERMEIER, Dept. of Mechanical and Nuclear Engineering, Penn State University, 129 Research East Building University Park, PA 16802, THOMAS L. REINECKE, Naval Research Laboratory, Washington, District of Columbia 20375, KIRILL A. VELIZHANIN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545 — Tunable functionalization of “all-surface” materials is a promising area of fundamental and applied research. Two-body interactions between adsorbed atoms or molecules on surfaces, such as graphene, are crucial to a variety of applications, ranging from transport to photovoltaics and DNA manipulations. We present our recent results for adsorbate-adsorbate interactions between mono-valent and between bi-valent adsorbates on graphene. These interactions are dominated by direct Coulomb coupling and exchange of itinerant electrons. A model Hamiltonian that encompasses different types of adsorbates is constructed and parameterized from ab initio density functional theory. The range of interactions is found to depend strongly on the local adsorbate-substrate bonding mechanism and on the chemical potential.

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