

Abstract Submitted
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Interactions between adsorbates on graphene DMITRY SOLENOV, CHAD JUNKERMEIER, THOMAS L. REINECKE, Naval Research Laboratory, Washington, District of Columbia 20375, USA, KIRILL A. VELIZHANIN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — Interactions between adsorbates on a surface of graphene play an important role in many applications. We offer a detailed analysis of interactions between two adsorbed atoms and molecules. We compare the first principles DFT, numerical tight-binding, and analytical functional integral calculations to identify the microscopic nature of the adsorbate-adsorbate interaction and the role of different contributions. The interaction has two distinct regimes: a weak coupling regime, which is akin to RKKY (Ruderman-Kittel-Kasuya-Yosida) magnetic interaction, and a strong coupling regime which is dominated by interaction via a many-body electronic dressing “cloud” around each adsorbate. We show that the interplay between these two regimes provides an opportunity to manipulate the magnitude and the structure of the adsorbate-adsorbate interaction (up to complete reversal of sign) via a variety of easily accessible properties, such chemical potential via back-gating, type of an adsorbed atom, electronic configuration of an adsorbed molecule, and strain.

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