

Abstract Submitted
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Adsorption of NH₂ on Graphene in the Presence of Primary Defects CHAD JUNKERMEIER, NRC Post-Doctoral Associate, U.S. Naval Research Laboratory, STEFAN BADESCU, U.S. Air Force Research Laboratory, THOMAS REINECKE, U.S. Naval Research Laboratory — The primary amine, NH₂, is of interest as a linker between graphene and organic molecules in novel biotechnologies using graphene platforms. We are using *ab initio* electronic structure calculations to study NH₂ adsorption on graphene. We find that the adsorption energy on pristine graphene is on the order of 0.778 eV, a relatively weak bond. We are interested in situations in which the bonding of NH₂ is stronger and are studying systems in which NH₂ adsorbs near defects. We find the adsorption energy of a NH₂ molecule near a second NH₂ molecule is as high as 1.037 eV and that the adsorption near a substitutional N atom is 1.063 eV. We find that there is a RKKY-like interaction between the adsorbate molecules in the case of two NH₂. We will also give results for NH₂ adsorption near other defects.

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