Recognition of DNA sequencing through binding of nucleobases to graphene   VALENTINA ZAFFINO, Univ of Central Florida — Graphene is one of the most promising materials in nanotechnology. Its large surface to volume ratio, high conductivity and electron mobility at room temperature are outstanding properties for use in DNA sensors. For this study, we used Density Functional Theory (DFT), ?with and without the inclusion of van der Waals (vdW) interactions, ?to investigate the adsorption of nucleobases (cytosine, guanine, adenine, thymine, and uracil) on pristine graphene and graphene with defects (Divacancy and Stone-Wales). We investigated the performance of two types of vdW-DF functional (optB86b-vdW and rPW86-vdW), as well as the PBE functional, and their description of the adsorption geometry and electronic structure of the nucleobase-graphene systems. The inclusion of defects results in an increase in binding energy, closer adsorption of the molecule to graphene and greater buckling in both the graphene structure and nucleobase.

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