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Van der Waals Interactions in Graphene Nanoribbons – Important Implications revealed via Theoretical Investigations

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Graphene nanoribbons (GNRs) are quasi-one dimenisional structures with planar geometry. They have extraordinary properties suitable for novel technological applications, especially for high speed electronics. Of particular importance is how GNRs interact with each other and other materials not only to understand their fundamental science, but also to help interpret experimental data and design better devices. Because of their inertness and nature of CC bonding, van der Waals (vdW) forces at small separations dominate GNR interactions. I will present studies revealing the collective microscopic nature of GNR vdW interactions based on a discrete dipole approximation. Calculations utilizing Density Functional Theory (DFT) with semi-empirical correction for the vdW interactions will also be presented for folded GNRs. In all cases, the emphasis will be on understanding the peculiarities of the vdW force in terms of registry dependence, strength, and role in mechanical manipulations involving GNRs. Furthermore, I will emphasize electronic structure modulations in terms of overall changes, energy gaps, magnetic states in various folded configurations as obtained via DFT.