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Scaling Laws for van der Waals Interactions in Nanostructured Materials VIVEKANAND GOBRE, ALEXANDRE TKATCHENKO, Fritz-Haber-Institut der MPG — Van der Waals (vdW) forces originate from interactions between fluctuating multipoles in matter and play a significant role in the structure and stability of nanostructured materials. Many models used to describe vdW interactions in nanomaterials are based on a simple pairwise-additive approximation, neglecting the strong electrodynamic response effects caused by long-range fluctuations in matter. We develop and utilize an efficient microscopic method [1,2]to demonstrate that vdW interactions in nanomaterials act at distances greater than typically assumed, and can be characterized by different scaling laws depending on the dimensionality and size of the system. Specifically, we study the behaviour of vdW interactions in single-layer and multilayer graphene, fullerenes of varying size, single-wall carbon nanotubes and graphene nanoribbons. As a function of nanostructure size, the van der Waals coefficients follow unusual trends for all of the considered systems, and deviate significantly from the conventionally employed pairwise-additive picture. We propose that the peculiar van der Waals interactions in nanostructured materials could be exploited to control their self-assembly. [1] Tkatchenko, DiStasio, Car, and Scheffler, PRL (2012); [2] Gobre, Tkatchenko, Nat. Commun. (2013).

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