Unusual Aspects of Dispersion Forces in Nanostructures

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There has been much recent progress in the ab initio description of dispersion forces between condensed-matter entities. In particular, empirical and non-empirical density functionals have been derived that produce both a reasonable short-ranged behavior and a reasonable asymptotic dispersion force, when applied to a wide variety of dimers where at least one component is a small molecule. They thus describe the whole van der Waals (vdW) interaction curve.

This talk will focus on dimers made from metallic or near-metallic nanostructures that are highly anisotropic, such as carbon nanotubes or graphene planes. In contrast to the case of bulk metals, the spontaneous long-wavelength electron density fluctuations on these systems are incompletely screened, leading to predictions of unusual dispersion forces that cannot be reproduced by any of the currently popular functionals. Cases will be discussed where not only the asymptotic force, but also the force at shorter distances (but still outside the regime of substantial electron cloud overlap) should be strongly different from the predictions of conventional vdW theories.