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Exploiting London dispersion forces in nonequilibrium growth of surface-based nanostructures¹

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London dispersion force describes the weak interaction between transient dipoles or multipoles associated with different parts of matter, and accounts for a major part of the attractive van der Waals (vdW) force. It is ubiquitous in nature, yet its importance in various physical and chemical processes just starts to be increasingly recognized. Such advances through definitive quantitative studies are largely enabled by the availability of more accurate descriptions of the weak interactions associated with long-range electron correlation effects within first-principles approaches. The present talk contains two parts, both obtained within the vdW-DF scheme on the theory side. In the first part, we critically assess the binding strengths of different classes of adatoms on ultrathin metal films of varying thicknesses. For inert gas atoms such as Xe, the London dispersion force is found to drastically enhance their adsorption, but the overall binding behavior depends only weakly on the film thickness. In contrast, for atoms with unpaired valence electrons such as H or O, the overall binding is much stronger, and also depends more sensitively on the film thickness, but with a much weaker and (in some cases) repulsive vdW contribution. These results have important implications in our developing a better understanding of atomic and molecular adsorption on different metal substrates. In the second part, we demonstrate unambiguously the decisive role of London dispersion force in non-equilibrium growth of ordered nanostructures on metal substrates using aromatic source molecules. Our multi-scale modeling integrating first-principles calculations with kinetic rate equation analysis shows that a drastic reduction in the growth temperature, from 1000°C to (250-300)°C, can be achieved in graphene growth on Cu(111) when the typical carbon source of methane is replaced by benzene or *p*-Terphenyl. The enhanced London dispersion forces effectively prevent easy desorption of the adsorbed molecules, facilitating their dehydrogenation, and promoting subsequent graphene growth at much lower temperatures. These strong predictions are further validated quantitatively in our experimental tests. We also demonstrate that the general trends established above are broadly applicable in graphene growth using other aromatic carbon sources.

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