Dipole Waves and van der Waals Interactions at the Nanoscale

Alexandre Tkatchenko University of Luxembourg, Luxembourg Email of Presenting Author: alexandre.tkatchenko@uni.lu

Recent experimental investigations of non-covalent forces at the nanoscale keep challenging the basic assumptions of widely employed particle- and fragment-based models for van der Waals (vdW) interactions and await an accurate and physically sound theoretical explanation. In this talk, I will argue that a qualitatively correct description of vdW interactions between polarizable non-metallic nanostructures over a wide range of finite distances can only be attained by accounting for the delocalized wavelike nature of electron density fluctuations. By considering a diverse set of nanoscale and biological systems with markedly different underlying dimensionalities, topologies, and polarizabilities, we find a visible enhancement in the non-locality of the charge density response on the range of 10--20 nm; furthermore, it is these collective wavelike fluctuations that are responsible for the emergence of non-trivial interaction power laws. The wavelike nature of vdW interactions provides a hitherto unexplored avenue towards understanding the structure and assembly of complex polarizable nanostructures.