Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Unifying microscopic and continuum treatments of van der Waals and Casimir interactions[1] PRASHANTH VENKATARAM, Princeton Univ, JAN HERMANN, Max Planck Gesellschaft, ALEXANDRE TKATCHENKO, University of Luxembourg, ALEJANDRO RODRIGUEZ, Princeton Univ — We present an approach for computing long-range, dispersive van der Waals (vdW) interactions between complex molecular systems and arbitrarily shaped macroscopic bodies, melding atomistic treatments of electronic fluctuations based on density functional theory (DFT) in the former, with continuum descriptions of strongly shape-dependent electromagnetic fields in the latter, thus capturing many-body and multiple scattering effects to all orders. Such a theory is especially important when considering vdW interactions at mesoscopic scales, i.e. between molecules and structured surfaces with features on the scale of molecular sizes, in which case the finite sizes, complex shapes, and resulting non-local electronic excitations of molecules are strongly influenced by electromagnetic retardation and wave effects that depend crucially on the shapes of surrounding macroscopic bodies. We show that these effects together can modify vdW interactions by orders of magnitude compared to previous treatments based on Casimir-Polder [1] or nonretarded [2] approximations, which are valid only at macroscopically large or atomic-scale separations, respectively. [1] J. F. Babb, J. Phys: Conf. Ser. 19, 1 (2005) [2] J. F. Dobson and T. Gould, J. Phys: Condensed Matter 24, 073201 (2012)

[1]NSF DGE 1148900, NSF DMR-1454836

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Date submitted: 10 Nov 2016 Electronic form version 1.4