

Abstract Submitted
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Strong van der Waals attractive forces in nanotechnology. JEFFREY REIMERS, Shanghai University / University of Technology Sydney — The Dobson classification scheme for failure of London-like expressions for describing dispersion is reviewed. New ways to measure using STM data and calculate by first principles free energies of organic self-assembly processes from solution will be discussed, considering tetraalkylporphyrins on graphite. How strong van der Waals forces can compete against covalent bonding to produce new molecular isomers and reaction pathways will also be demonstrated, focusing on gold-sulfur bonds for sensors and stabilizing nanoparticles. (1) Reimers, J. R.; Goerigk, L.; Ford, Elemans, J. A. A. W.; Hush, N. S.; Crossley, M. J. et al "A priori calculations of the free energy of formation from solution of polymorphic self-assembled monolayers" *Proc. Natl. Acad. Sci. U.S.A.* **2015**, *112*, E6101. (2) Reimers, J. R.; Ford, M. J.; Halder, A.; Ulstrup, J.; Hush, N. S. "Gold surfaces and nanoparticles are protected by Au(0)-thiyl species and are destroyed when Au(I)-thiolates form" *Proc. Natl. Acad. Sci. U.S.A.* **2016**, *113*, E1424. (3) Reimers, J. R.; Li, M.; Wan, D.; Gould, T.; Ford, M. J. In *Noncovalent interactions in quantum chemistry and physics: Theory and applications*; Otero de la Roza, A., DiLabio, G., Eds.; Elsevier: Amsterdam, 2017, p in press.

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