



IBS Center for Multidimensional Carbon Materials



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van der Waals Effects in van der Waals Materials

OCT 13 | Bldg. 101
FRI 16:00 | Seminar Room on the 1st floor

The influence of van der Waals interactions extends well beyond binding energies and encompasses the structural, mechanical, spectroscopic, and even electronic signatures of molecular systems and condensed matter [1]. However, our conceptual understanding of these ubiquitous interactions is largely based on perturbative models, which are often unable to capture the full extent of non-local quantum-mechanical fluctuations which can extend up to tens of nanometers in real systems [2]. Here we present and analyze a few remarkable and rarely recognized aspects of vdW interactions:

- (1) Their ultra-long range in polarizable molecules and materials [1,2,3],
- (2) Their tunability by applied electric fields,
- (3) Their marked influence on observable electronic properties of materials [4],
- (4) The possibility to make vdW interactions repulsive for confined molecules [5].

The development of efficient many-body methods that explicitly address the non-local collective nature of vdW interactions not only leads to significant improvements in the accuracy of calculations [6,7,8] but also allows us to discover novel conceptual insights that give us the ability to control these interactions in the design of intricate materials. These facts will be highlighted by presenting a few selected examples from our recent work [1,7,8].

- [1] J. Hermann, R. A. DiStasio Jr., and A. Tkatchenko, *Chem. Rev.* 117, 4714 (2017).
- [2] A. Ambrosetti, N. Ferri, R. A. DiStasio Jr., and A. Tkatchenko, *Science* 351, 1171 (2016).
- [3] J. Hermann, D. Alfe, and A. Tkatchenko, *Nature Commun.* 8, 14052 (2017).
- [4] N. Ferri, R. A. DiStasio Jr., A. Ambrosetti, R. Car, and A. Tkatchenko, *Phys. Rev. Lett.* 114, 176802 (2015).
- [5] M. Sadhukhan and A. Tkatchenko, *Phys. Rev. Lett.* 118, 210402 (2017).
- [6] A. Tkatchenko, R. A. DiStasio Jr., R. Car, and M. Scheffler, *Phys. Rev. Lett.* 108, 236402 (2012).
- [7] A. Tkatchenko, *Adv. Func. Mat.* 25, 2054 (2015).
- [8] A. M. Reilly and A. Tkatchenko, *Chem. Sci.* 6, 3289 (2015).

You are cordially invited to attend!

Special Guest Speaker