20 Dec **Monday** **12:45 – 1:30** **Chair: YANG Shengyuan (杨声远)**

Prominent Nonequilibrium Effects in Nanoscale Electronic Devices Predicted by Steady-State DFT

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Professor ZHANG Chun graduated from Fudan University in 1996 with B.S. (applied physics) and in 2000 with M.S. (physics). After obtaining his Ph.D in computational condensed matter physics in 2004 at University of Florida, he worked as a postdoc research fellow from 2005 to 2008 in school of physics at Georgia Institute of Technology. He then joined National University of Singapore as an assistant professor in Department of Physics and Department of Chemistry, and was promoted to associated professor in 2015. Dr. Zhang's research interests include development of first-principles theories for quantum systems under various conditions, theoretical design of low-dimensional materials, electron quantum transport at molecular scale, and catalysis at nanoscale or atomic scale. Professor Zhang has published 90+ papers in main-stream journals in computational condensed matter physics and quantum chemistry (PRL, JACS, Nature Series, Adv. Mater., PRB, APL, JCP etc.) that have been cited 7000+ times.

Abstract:

The standard density functional theory (DFT) based computational approach has been widely used in past two decades in theoretically studying transport properties of nanoscale (or molecular scale) devices under a finite bias. A recent experiment[1], however, reported surprising transport phenomena in silanes molecules that cannot be understood by the standard DFT approach, presenting a serious challenge for the community of computational nanoscience. With the steady-state DFT (SS-DFT)[2] we recently proposed, we found that underlying the 'puzzling' transport properties of silanes molecules is a novel type of bias-induced nonequilibrium effects (named 'nonequilibrium pulling' in our work)[3]. Our calculations show that when the system is near equilibrium, the standard DFT approach is a good approximation of SS-DFT, while the 'nonequilibrium pulling' could drive the silanes molecules far away from the equilibrium at low biases around 0.2 V, causing the failure of the standard DFT approach and the experimentally observed surprising transport phenomena. Detailed analysis suggests that the nonequilibrium effects we predicted may generally exist in nanoscale junctions when there are conducting channels that are close to the bias window and mainly residing at the source contact. These findings significantly broaden our fundamental understanding of electron quantum transport at nanoscale.

References
[1] H. Li et. al, *Angew. Chem. Int. Ed.*, **2017**, 56, 14145.
[2] S. Liu, A. Nurbawono and C. Zhang, *Sci. Rep.*, **2015**, 5, 15386.
[3] Z. Jiang, KM. Yam, N. Guo, L. Zhang, L. Shen and C. Zhang, *Nanoscale Horiz.*, **2021**, 6, 801.