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Mesoscopic and nanoscopic physics of molecular-scale electronics YONGQIANG XUE, SUNY-Albany — Going from the mesoscopic regime of quantum semiconductor device to nanoscopic molecular device, the dominant or first-order transport mechanism remains quantum mechanical coherent transport due to the small size. A large part of the theoretical efforts in nanoelectronics is thus to recast the accumulated knowledge about mesoscopic physics into forms that are suitable for evaluating quantum transport phenomena at the atomic-scale. On the other hand, electrical conduction is intrinsically a dynamical phenomenon. Since the different degrees of freedom (electronic, mechanical, phonon…) in the nanostructures can be strongly coupled to each other and to their nano-environment, the measured electrical signal is often the result of complex dynamic coupling processes without requiring ensemble average. New theoretical principles and computational techniques may be needed to unravel the rich physics involved in molecular-scale transport. In this talk, we discuss our efforts in moving from mesoscopic theory to nanoscopic theory of molecular-scale electronics.

Yongqiang Xue
SUNY-Albany

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