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# *Quantum Transport in Molecular Wires*

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Molecule-based electronics holds substantial promise for quite a range of practical applications. Molecular devices operate by principle of quantum mechanics, their properties are closely related to the atomic and molecular structure of the system. It has been a very difficult problem to calculate these properties including relevant microscopic details without any phenomenological parameter. In this seminar, I will discuss recent progress in theoretical modeling of quantum transport from atomic first principles. I will then report our recent investigation on transport properties of molecular wires and compare results to the corresponding experimental data. I will conclude by discussing some general trends we have learned on electronic conduction at the molecular scale.

**Hong Guo** obtained his Ph.D degree in theoretical condensed matter physics from the University of Pittsburgh in 1987. He came to McGill University in 1989 and is now a James McGill Professor of Physics. His research interests are in the field of mesoscopic physics, quantum transport theory, nanoelectronic device physics, molecular electronics, nonequilibrium phenomena, density functional theory, strongly correlated electrons in low dimensional nanostructures, computational physics and various topics of materials theory.