



Monday, November 06, 2017, 12:00 pm

Seaver Science Library, Room 150

SSC Auditorium next to the library

Professor Ignacio Franco

Department of Chemistry

University of Rochester

Atomistic Modeling of Electromechanical Spectroscopies in Molecular Junctions

Abstract:

In this talk I will summarize theoretical and computational efforts that aim at bringing theory and experiment closer together in molecular electronics, and at developing the capabilities to atomistically understand experiments that simultaneously measure the electric and mechanical properties of single-molecules in the context of nanoscale junctions. Developing atomistic understanding through simulations is essential to advance this class of measurements into a highly discriminating multidimensional single-molecule spectroscopy.

Reliability in molecular electronics experiments has come from statistically sampling thousands of repeat measurements. Thus, a great challenge for simulations is to correctly capture the statistical variations in molecular conformation, junction geometry and transport properties observed in and between experiments. To obtain meaningful statistics, it is necessary to describe both the dynamics and the transport using accurate and computationally efficient methods. I will describe recent developments that advance our ability to model and understand electromechanical processes in molecular junctions. Specifically, I will introduce well-defined conditions for the validity of steady-state approximations to time-dependent currents, accurate classical force field for non-reactive metal-molecule interactions, and strategies to model these experiments with statistics. I will also illustrate the utility of this class of experiments as a multidimensional single-molecule spectroscopy through examples across the chemical spectrum.

Suggested Reading:

Carey, R.; Chen, L.; Gu, B.; Franco, I. *The Journal of Chemical Physics* **2017**, *146*(17), 174101.

Pirrotta, A.; Vico, L. D.; Solomon, G. C.; Franco, I. *The Journal of Chemical Physics* **2017**, *146*(9), 092329.

Hosted by Professor Anna Krylov

The scientific community is invited

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