



**BENEMÉRITA UNIVERSIDAD AUTÓNOMA
DE PUEBLA**
INSTITUTO DE FÍSICA “Ing. Luis Rivera Terrazas”
SEMINARIO SEMANAL “Jesús Reyes Corona”



“First principles numerical modeling of electronic, optoelectronic and photonic devices”

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RESUMEN: Matrix quantum kinetics has been highly impactful in first principles as well as phenomenological modeling of a variety of transport phenomena, such as electron flow through conventional semiconductors, organics or 2-D materials, thermoelectric and thermal conductivity, and spin torque. I will introduce the Keldysh Non-Equilibrium Green's Functions (NEGF) formalism that can cover both Landauer type quantum flow, as well as Boltzmann type semi-classical conduction in presence of incoherent scattering. Starting with a simple 'toy' model of two contacts and a barrier channel material, we will show we can progressively go into parameter-free, quantum chemistry models for electronic current and conductance. We will then expand to spin currents and nonequilibrium spin Hall/spin torques in magnetic materials. Expanding the Fermi surface over a frequency range extends this description to optical conductivity, while higher order expansions go into nonlinear photogalvanic effects. Finally, adding suitable scattering self-energies extends this approach to strongly nonequilibrium properties such as impact ionization. We thus have an atom-to-system predictive and practical toolkit that can be used to design emerging logic, memory, and sensor applications.

Auditorio del Instituto

Viernes 6 de marzo de 2026

13:00 hrs