1st European Workshop of Open Quantum Systems

EWOQS 2026

BOOK OF ABSTRACTS

15-17 June 2026

Universidad Politécnica de Cartagena (Spain)

01
ABSTRACT

Quantum Dynamics of Charges in Organic Semiconductors: Insights from Hierarchical Equations of Motion

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Abstract

The motion of a charge carrier in high-mobility organic semiconductors is mainly limited by its moderate coupling to slow and abundantly thermally excited intermolecular vibrations [1]. Optical conductivity is then dominated by the displaced Drude peak [2], which can be understood by assuming Newtonian [3,4] or some effective vibrational dynamics [2]. However, fully quantum dynamical insights into long-distance charge transport remain elusive, even in the one-dimensional Peierls model featuring a single vibration per lattice site.

In this contribution, we present our numerically exact hierarchical equations of motion (HEOM)-based framework to compute transport properties of the one-dimensional Peierls model [5,6]. The correlation functions involving the phonon-assisted current are handled using our novel explicit expression of HEOM auxiliary operators in terms of creation and annihilation operators of vibrational quanta [5]. We find that the displaced Drude peak is accompanied by an optical-conductivity enhancement below vibrational frequency [6], which is not observed in experimental low-frequency signatures. We then consider a more realistic model with a continuous distribution of vibrational modes mimicked by the Brownian-oscillator spectral density, and solve it using the dissipaton equations of motion [7]. We observe that the optical-conductivity enhancements at very low frequencies disappear already in the underdamped-oscillator regime [7], meaning that the enhancement reported in [6] is an artifact of the assumed delta-like distribution of vibrational modes.

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This research is supported by the Science Fund of the Republic of Serbia, Grant No. 5468, Polaron Mobility in Model Systems and Real Materials – PolMoReMa.

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