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The Molecular Photo-Cell: Quantum Transport and Energy Conversion at Strong Non-Equilibrium SHIGERU AJISAKA, Department of Chemistry, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel, BOJAN ZUNKOVIC, Departamento de Física, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Casilla, JONATAN DUBI, Department of Chemistry, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel — The molecular photo-cell is a single molecular donor-acceptor complex attached to electrodes and subject to external illumination. Besides the obvious relevance to molecular photo-voltaics, the molecular photo-cell is of interest being a paradigmatic example for a system that inherently operates in out-of-equilibrium conditions and typically far from the linear response regime. Moreover, this system includes electrons, phonons and photons, and environments which induce coherent and incoherent processes, making it a challenging system to address theoretically. Here, using an open quantum systems approach, we analyze the non-equilibrium transport properties and energy conversion performance of a molecular photo-cell, including for the first time both coherent and incoherent processes and treating electrons, photons, and phonons on an equal footing. We find that both the non-equilibrium conditions and decoherence play a crucial role in determining the performance of the photovoltaic conversion and the optimal energy configuration of the molecular system.

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