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Visualizing electron dynamics in organic materials: Charge transport through molecules and angular resolved photoemission[1]

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Being able to visualize the dynamics of electrons in organic materials is a fascinating perspective. Simulations based on time-dependent density functional theory allow to realize this hope, as they visualize the flow of charge through molecular structures in real-space and real-time. We here present results on two fundamental processes: Photoemission from organic semiconductor molecules [1] and charge transport through molecular structures [2]. In the first part we demonstrate that angular resolved photoemission intensities - from both theory and experiment - can often be interpreted as a visualization of molecular orbitals. However, counter-intuitive quantum-mechanical electron dynamics such as emission perpendicular to the direction of the electrical field can substantially alter the picture, adding surprising features to the molecular orbital interpretation. In a second study we calculate the flow of charge through conjugated molecules. The calculations show in real time how breaks in the conjugation can lead to a local buildup of charge and the formation of local electrical dipoles. These can interact with neighboring molecular chains. As a consequence, collections of "molecular electrical wires" can show distinctly different characteristics than "classical electrical wires".

1. M. Dauth et al., Physical Review Letters **117**, 183001 (2016)
2. P. Schaffhauser, S. Kümmel, Phys. Rev. B **93**, 035115 (2016)

[1]German Science Foundation GRK 1640