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Kinetic model of the formation of STM-induced electrofluorochromism in molecular junctions

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Experimental data on STM-induced electroluminescence in monomolecular junctions have led to the need to elucidate the physics of the formation of optoelectronic processes at the atomic-molecular level, taking into account both dynamic and relaxation processes. A mechanism for the formation of electrofluorochromism based on a kinetic model has been proposed [1]. In this model, the description of the optoelectronic process in a photoactive molecular junction takes into account the fact that the formation of electron current and electroluminescence (EL) is controlled not only by the shift of the orbital energies of the molecule relative to the Fermi levels of both electrodes, but also by the probability of the realization of many-body states of the molecule at different values and polarities of the bias voltage. Therefore, when current and EL are generated, the electronic states of charged forms of fluorophore molecules can act not only as mediators of electron transfer, but also become responsible for electrofluorochromism. It became clear that the EL in a molecular junction reflects the light emission of a fluorophore molecule not only between the singlet states of a neutral molecule, but also between the states of its charged forms. Thus, we show that electron transfer occurs through the transmission channels associated with electronic states of the neutral molecule and its cationic and anionic forms, which, at a definite bias voltages, are involved in electron transfer. The occupancies of these states are determined by kinetic processes in the molecular junction and therefore depend on the ratio of charge exchange rates between the molecule and the electrodes, the rates of non-radiative intramolecular transitions caused by inelastic interelectrode tunneling of electrons, as well as the rates of intramolecular radiative transitions enhanced by the plasmonic response. Analytical results are obtained using the tight-binding Hamiltonian for a molecule. The kinetic model made it possible to explain the features of EL in a monomolecular junction with the ZnPc fluorophore. Thus, it was shown that the description of EL based on the kinetic approach can serve as an effective tool for understanding the physics of optoelectronic processes in single-molecule structures.

1. E.Petrov, O.Kapitanchuk, Ye.Shevchenko, V.Gorbach, A.Lyubchik, Phys. Chem. Chem. Phys., 2024, DOI: 10.1039/d4cp01328j

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