Nanooptics and photonics

Electroluminescence of single molecule between macroscopic electrodes

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A transformation of the energy of the moving charges into the energy of light would mainly depends on an energy gap between the HOMO/LUMO levels and the electrodes Fermi levels. Recent studies show that a luminescence had been observed only if a voltage bias exceeds an energy gap between the HOMO and the LUMO levels. However, the mechanisms of regulation of molecular electroluminescence need detail theoretical investigation. In the work [1], we study how the transmission gaps in the system “electrode 1-molecule-electrode 2” affect the formation of fluorescence and phosphorescence and how this phenomenon depends on the voltage bias.

We have demonstrated that there is two mechanisms of molecule excitation during the interelectrode charge transfer and, thus, formation of the electroluminescence. The first one (sequential electron hopping) consist of electron jumps between the molecule and the electrodes. The two consecutive electron jumps can leave a molecule in the excited state. The hopping mechanism is the most effective at such voltage bias when a resonant regime is switched on for the electron transmission. This means that an electron can jump from one of the electrodes onto the molecule without activation. During the second mechanism (related to a direct inelastic electron tunneling) the charged molecular state participates in electron transport in a virtual manner. In this case, the bias must exceed the difference between ground and excited molecular states. We have shown that fluorescence and phosphorescence frequencies can depend on the applied voltage bias despite their intensity don’t depend on the bias anymore. This effect is expected to occur for molecules with considerably different distribution of electron densities within the HOMO and the LUMO.

1. *Leonov V. O., Shevchenko Ye. V., Petrov E. G.* Formation of Electroluminescence in an Electrode–Molecule–Electrode System // Ukr J Phys.-2014.-**59**, N 6.-P. 628.