Molecular doping of nucleic acids into light emitting crystals driven by multisite-intermolecular interaction

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We reveal the fundamental understanding of molecular doping of DNAs into organic semiconducting tris (8-hydroxyquinoline) aluminum (Alq3) crystals by varying types and numbers of purines and pyrimidines constituting DNA. Electrostatic, hydrogen bonding, and π-π stacking interactions between Alq3 and DNAs are the major factors affecting the molecular doping. Longer DNAs induce a higher degree of doping due to electrostatic interactions between phosphate backbone and Alq3. Among four bases, single thymine bases induce the multisite interactions of π-π stacking and hydrogen bonding with single Alq3, occurring within a probability of 4.37%. In contrast, single adenine bases form multisite interactions, within lower probability (1.93%), with two-neighboring Alq3. These multisite interactions facilitate the molecular doping into Alq3 particles compared to cytosines or guanines only forming π-π stacking. Thus, photoluminescence and optical waveguide phenomena of crystals were successfully tailored. This discovery should deepen our fundamental understanding of incorporating DNAs into organic semiconducting crystals.