Theoretical modeling in nanophotonics

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Several books have been published recently on various aspects of nanophotonics [1–4], and one of them [4] is fully devoted to organic nanophotonics. However, as strange as it may seem, molecular aspects of organic nanophotonics are almost not considered in [1–4]. Consequently, such important problems as molecules and molecular complexes, their structure, light absorption and emission, intermolecular charge and energy transfer in disordered organic functional layers, and calculations of the corresponding parameters remained outside the scope of [1–4]. This lecture is specially devoted to theoretical and computational aspects of these problems. Some of them were briefly considered in [5]. However, the main focus in [5] was on the simulation of nanophotonics structures. On the contrary, this lecture is devoted to modern quantum-chemical methods specially designed recently and currently used in the calculations of parameters required for the best description of excited states in organic molecules and in their intermolecular complexes (exciplexes), which are often characterized by significant intra- and intermolecular charge transfer. The set of these parameters include geometrical (structural) parameters and energy data for ground and excited states, charge and energy transfer parameters, light absorption and emission characteristics, and related properties.

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References

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