Abstract

Chromophores Supramolecular Organization in Polymer Materials with Quadratic Nonlinear-Optical Activity: Symmetry Aspects †

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Organic dipole chromophores incorporated into a polymer matrix serve as molecular sources of its nonlinear-optical (NLO) activity. To exhibit quadratic NLO response, polymer material should be noncentrosymmetrical; this is achieved by the chromophores’ orientation in the applied electric field. Atomistic modelling of oligomers with covalently bound chromophores revealed the formation of stacked structures formed by chromophores with codirected dipole moments, in which two to four chromophores participate. The chromophores in the stacks are shown to be mutually shifted; the shift value determines the NLO characteristics of such structures. Another approach to the supramolecular organization of chromophore groups in the material is realized via Hydrogen bonds with the formation of the so-called J-dimers composed of chromophores, which results in the considerable growth of the NLO characteristics of the material. Thus, the formation of supramolecular aggregates could contribute to the optimization of the optical nonlinearity of the material.

Vibrational spectroscopy provides the tool to monitor the presence of such aggregates. The comparison of experimental and quantum-chemically calculated spectra permits separate chromophores, H-dimers with different structures and J-dimers to be revealed in the material, and provides guidelines for the design of chromophores that are effective for the realization of materials with high quadratic NLO activity.

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