Ab initio calculations of nonlinear polarizabilities of fullerene-porphyrin complexes

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Nonlinear optical properties of *M*TPP and C_{60}-*M*TPP complexes (*M*=H_2, Zn, Cu; TPP – tetraphenylporphyrin) are studied. Accurate ab initio calculations of electronic structure, optimized geometry, static linear and nonlinear polarizabilities (including first and second order hyperpolarizabilities) of C_{60}, *M*TPP molecules and C_{60}-*M*TPP complexes have been carried out using DFT/B3LYP method. It is shown that C_{60} and *M*TPP form a stable charge transfer complex C_{60}-*M*TPP, resulting in a giant enhancement of the nonlinear response. It is found that the enhancement of optical nonlinearity is not necessarily connected with the formation of covalent bonds between the components. The work is supported by Russian Foundation for Basic Research (Grant № 09-02-01008).