Comparison of ab initio HF and DFT calculations of the structure and spectroscopy of two dimeric systems of chloro Yb(III) mono-phthalocyanine in polymeric lattice.

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Streszczenie

Lanthanide complexes with phthalocyanines (Pc) and porphyrins are of great interest because of their unique luminescence behavior and many applications. Our research is devoted to photophysical studies and theoretical calculations HF and DFT of the structure and spectroscopy of two dimeric systems, created by chloro Yb(III) monophthalocyanines and comparison of the calculated spectroscopic behaviour with the experimental one for monomeric chelate in polymeric lattice of PMMA.

Ytterbium chelates were chosen because they have special properties appropriate for technology of different materials with unique spectroscopic behaviour in NIR region, which is not overlapped by very intensive emission of π-conjugated system of phthalocyanine or by upconversion transitions.

The drastic variation in emission properties of materials depend on the energy of excitation, and only minor changes are observed in spectroscopic frequencies of dimeric systems compared to monomeric ones. Attention is paid to the radiative, non-radiative and non-linear processes, intramolecular energy transfer and the role of charge-transfer state in this process.

Słowa kluczowe

Ytterbium, Monophthalocyanine, DFT and Ab initio HF calculation, Spectroscopic properties, Dimeric systems, Spectroscopy in polymeric matrix

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