

研究论文

双核金属茂合物 $Zn_2(\eta^5-E_5)_2$ ($E=N, P, As, Sb$) 电子结构和三阶非线性光学性质的理论研究

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摘要 运用密度泛函PBE0方法研究了双核金属茂合物 $Zn_2(\eta^5-E_5)_2$ ($E=N, P, As, Sb$)的电子结构, 运用自然键轨道(NBO)方法对该体系的电荷分布及成键特征进行了分析. 此类体系中存在Zn—Zn的 σ 单键, 为近似纯s成分的成键方式. 用含时密度泛函理论(TDDFT) 完全态求和(SOS) 方法计算了该体系的三阶非线性光学系数, 结果表明, γ 值与最大吸收波长 λ_{max} 成正比, 在各个分量中, 对 $\langle \gamma \rangle$ 起主要贡献的是 γ_{zzzz} , 最大吸收波长对应的电子跃迁是从Zn—Zn的 σ 成键轨道到Zn—Zn的 σ^* 反键轨道.

关键词 [双核金属茂合物](#) [非线性光学性质](#) [自然键轨道](#) [含时密度泛函理论](#) [态求和方法](#)

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Theoretical Studies on Electronic Structures and Third-order Nonlinear Optical Properties of Di-metallocene Complexes $Zn_2(\eta^5-E_5)_2$ ($E=N, P, As, Sb$)

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Abstract Electronic structures of di-metallocene complexes $Zn_2(\eta^5-E_5)_2$ ($E=N, P, As, Sb$) were investigated with DFT PBE0 method. Charge distribution and bonding characters are analyzed with Natural Bond Orbital(NBO) Theory. The results show that a single σ -bond of Zn—Zn exist in these complexes with a nearly pure s character. The nonlinear third-order polarizabilities (γ) were calculated for the four di-metallocene complexes by time-dependent density functional theory(TD-DFT) combined with sum-over-states(SOS) method. The calculated results show that γ value is in direct proportion to the maximum absorption wavelength(λ_{max}). Analysis of the main contributions to the third-order polarizability suggests that electron transfer(Zn—Zn σ -bond \rightarrow Zn—Zn σ^* -bond) along z-axis direction plays a key role in the nonlinear optical response.

Key words [Di-metallocene complexes](#) [NLO property](#) [NBO](#) [TD-DFT](#) [SOS method](#)

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