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化学

HPuO分子激发态的外场效应

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摘要 采用密度泛函(DFT)方法B3LYP/Gen，在Pu为相对论有效原子实势(RECP)基组水平上，优化计算得到了分子轴方向不同电偶极场（－0.005～0.005 a.u.）作用下的HPuO的基态几何结构、偶极矩和分子总能量。在优化构型下，用同样的基组，采用含时密度泛函(TDDFT)方法(TD-B3LYP)，研究了同样外电场条件下对HPuO的激发能的影响。计算结果表明，在外场作用下，对HPuO的前5个激发态电子跃迁光谱属于红外远红外光谱，波长为1 046.0～3 038.7 nm，这是钚原子的奇异特征。激发能与外电场的关系近似满足Grozema等提出的关系。

关键词 HPuO 激发态 电偶极场 含时密度泛函

分类号

Effect of External Electric Field of Excited State for HPuO

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Abstract The ground state of HPuO under different electric fields ranging from －0.005 to 0.005 a.u. was optimized using density functional theory DFT/B3LYP with relativistic effective core potential (RECP) for Pu and 6-311+G* for O and H. The excitation energy was calculated under the same electric fields employing the time-dependent DFT method. The results show that the electronic state, total energy, molecular geometry, dipole moment and excitation energy are strongly dependent on the field strength of applied electric field. The dependence of the calculated excitation energy on the applied electric field strength is fitting well to the relationship proposed by Grozema. The spectra of the first five excited electrons of HPuO are in the regions of infrared-far infrared. The wavelength is in the range of 1 046.0-3 038.7 nm.

Key words HPuO excited state dipole electric field time-dependent

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