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MX~4(M=Ti,Zr,Hf;X=Cl,Br)的电子结构研究

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摘要 本文利用单电子非相对论Hartree-Fock-Slater和完全相对论Dirac-Fock-Slater两种离散变分局域密度泛函方法(DV-Xα), 对MX~4(M=Ti,Zr,Hf;X=Cl,Br)的电子基态和相应于低能UV光谱的激发态进行了计算, 结果与实验符合得较好。用Mulliken布居分析方法研究了分子的共价性质, 发现除HfBr~4外, 相对论效应对金属与配体之间的键级影响很小。

关键词 电子结构 钛化合物 锆化合物 共价键 铪化合物 相对论效应

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Studies on the electronic structures of MX~4(M=Ti,Zr,Hf; X=Cl,Br)

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Abstract Molecular-orbital calculations on the ground states and optical excitation states corresponding to low energy valence UV spectra of MX~4(M=Ti,Zr,Hf;X=Cl,Br) have been carried out using both self-consistent one-electron nonrelativistic Hartree-Fock-Slater and fully relativistic Dirac-Fock-Slater discrete variational local-density functional methods within the self-consistent multipolar (SCM) charge density framework. The present results are in closer agreement with experiments than other theoretical calculations. The covalent bonding characters of the molecules are also investigated by means of Mulliken population analysis methods. The overlaps between metal and ligands for the molecules are insensitive to the relativistic effects except HfBr~4.

Key words ELECTRONIC STRUCTURE TITANIUM COMPOUNDS ZIRCONIUM COMPOUNDS COVALENT BONDS HAFNIUM COMPOUNDS

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