

稀土夹心化合物的SCF-X- α -SW研究 I: Cp~2Sm, Cp~2Yb 和 Cp~3Sm

闵新民

武汉工业大学新材料研究所

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摘要 对Cp~2Sm、Cp~2Yb和Cp~3Sm进行了非相对论和相对论SCF-X- α -SW计算,用轨道相互作用、分子轨道图形、布居数分析等方法讨论了化学键图象。在Cp~2Ln(Ln=稀土元素)中以Cp为主要成分的轨道能级两种方案结果变化不大。而相对论间接效应的存在,使Ln4f能级明显升高,与Cp~2Ln易被氧化的实验结果一致。二价的Cp~2Ln成键轨道中Ln成分是d>f>p>s,与三价的Cp~3Sm、LnF~3比较,Ln的s、p、d成分变化不大,而Ln f成分明显减少,使Cp~2Ln共价性明显地低于Cp~3Sm和LnF~3。

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SCF-X- α -SW Calculations on lanthanide metallocenes I: Cp~2Sm, Cp~2Yb and Cp~3Sm

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Abstract SCF-X- α -SW calcns. are carried out on Cp2Sm, Cp2Yb and Cp3Sm; both the nonrelativistic and relativistic schemes have been tried. The bonding pictures are discussed from interactions of the orbitals, the orbital maps and the populations. In Cp2Ln (Ln = Lanthanide) there are little differences in the levels of which orbitals involve dominantly Cp components between the two schemes, but due to relativistic indirect effect, Ln 4f level rises up notably, which is consistent with the experimental results that Cp2Ln is easily oxidized. Ln orbital components for the bonding orbitals of Cp2Ln are in the order d>f>p>s, those of Cp3Ln are f>d>p>s. Comparing each other, s, p and d components vary a little bit but f one decreases in Cp2Ln. Therefore the covalent bonding strength of Cp2Ln is evidently weaker than those of Cp3Sm and LnF3.

Key words [CALCULATION](#) [CYCLOPENTADIENE](#) [MOLECULAR ORBIT](#) [CHEMICAL BONDS](#) [RARE EARTH COMPOUNDS](#) [RELATIVITY THEORY](#) [NONRELATIVISTIC SCHEME](#)

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