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放热型金属合金化对钒基贮氢材料性能影响的理论研究

Theoretical Investigation on the Effect of Exothermic Alloying on Storage Hydrogen Materials

中文关键词：钒基贮氢材料；放热型金属；合金化；离散变分Xα方法

英文关键词：vanadium based hydrogen storage materials; exothermic metal; alloying; SCC-DV-Xα method

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作者	单位
李 荣	重庆师范大学化学学院，重庆 400047；重庆大学材料科学与工程学院，重庆 400044
周上祺	重庆大学材料科学与工程学院，重庆 400044
梁国明	重庆师范大学化学学院，重庆 400047
罗小玲	重庆师范大学化学学院，重庆 400047

中文摘要：

利用电荷自洽离散变分Xα(SCC-DV-Xα)方法计算了放热型金属合金化对钒基贮氢材料性能的影响。研究结果表明:在钒氢化物$V_{63}H_{64}$中加入放热型金属后，钒原子的净电荷都减少，而氢原子的净电荷既有增加又有减少，加入Ti、Ca以后，H原子的净电荷减少，而加入Mg、Zr以后，H原子的净电荷增加。研究还表明放热型金属合金化以后，V4*s*轨道电子态密度峰发生分裂，与H1*s*和H2*s*轨道电子态密度重叠程度增大，V-H之间相互作用增强;差分电荷密度还表明M-H之间也有较强的相互作用。Mg合金化导致氢化物$V_{51}M_{12}H_{64}$的费米能增加，氢化物稳定性减弱;Ca、Ti、Zr合金化导致氢化物$V_{51}M_{12}H_{64}$的费米能减少，氢化物更稳定。

英文摘要：

The effect of exothermic alloying on Vanadium-based hydrogen storage materials is calculated by the method of Xα (SCC-DV-Xα) cluster. The calculated results show that: when the exothermic metal is added into $V_{63}H_{64}$, the net charge of V decreases, on the other hand, the net charge of H decreases when Ti or Ca is added into $V_{63}H_{64}$, while it increases by adding of Mg or Zr into $V_{63}H_{64}$. Moreover, with the alloying of exothermic metal, the density peak of V4*s* orbital breaks up. And the V4*s* orbital overlaps with H1*s* and H2*s* more in exothermic alloyed materials than in unalloyed $V_{63}H_{64}$, which demonstrates that the ionic interaction between V and H strengthens. And, the charge density difference indicates strong interaction between the alloying metal M and H in $V_{51}M_{12}H_{64}$. The Fermi energy of $V_{51}M_{12}H_{64}$ is higher than unalloyed $V_{63}H_{64}$, which displays that the hydride becomes more unstable by adding of Mg. Oppositely, the Fermi energy of the hydride falls down by adding of Ca, Ti, Zr, thus $V_{51}M_{12}H_{64}$(M=Ca, Ti, Zr) are more stable than unalloyed $V_{63}H_{64}$.

主办单位：中国化学会　单位地址：南京大学化学楼

服务热线：(025)83592307　传真：(025)83592307　邮编：210093　Email：wjhx@netra.nju.edu.cn

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