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金属Mg晶格稳定性的第一原理电子结构计算

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摘 要： 采用最小二乘法对SGTE纯单质数据库中金属Mg的Gibbs能表达式进行了重新评估，得到了比SGTE数据库更精确的结果；同时，将SGTE数据库的晶格稳定参数外推至0 K，与第一原理总能赝势平面波方法的结果进行了对比，发现第一原理的晶格稳定参数结果为$\Delta G^{bcc-hcp}>\Delta G^{fcc-hcp}>0$，与SGTE外推结果一致。同时，研究还发现：第一原理总能平面波赝势方法计算的hcp-、fcc-和bcc-Mg的晶格常数和原子体积比实验值以及投影缀加波方法得到的结果偏大，结合能出现了完全相反的结果，并且3种结构的部分s态电子转化为p态电子形成了更强的化学键。

关键字： Mg；Gibbs能；电子结构；晶格稳定性；第一原理

Calculations of lattice stabilities of elemental Mg from electronic structures in first principles

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Abstract: The correction of transition data and reassessment of the parameters of Gibbs energy of elemental Mg were performed with the least-square method and the results agree more accurately with JANAF data than those of SGTE database. At the same time, the lattice stability parameters obtained by CALPHAD method in SGTE database were extrapolated to 0 K, and these results were compared with those of total energy plane wave pseudopotential method in first principles. It is found that the result of first principles agrees completely with that of SGTE, $\Delta G^{bcc-hcp}>\Delta G^{fcc-hcp}>0$. Besides, it is found that the results of lattice constants and atomic volumes of hcp-, fcc- and bcc-Mg calculated by total energy plane wave pseudopotential method are much larger than experimental data and those of projector augmented wave method in first principles. The contrary case occurs in total energy. And part of s state electrons in atoms were changed into

p state electrons in crystals to form stronger chemical bonding.

Key words: Mg; Gibbs energy; electronic structure; lattice stability; first principles

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