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# $MoSi_2$和$WSi_2$电子结构及光学性质的数值研究

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摘 要：应用基于密度泛函平面波赝势方法(PWP)，考虑广义梯度近似(GGA)下的交换关联势，计算具有$C11_b$型体心立方结构的$MoSi_2$和$WSi_2$单晶的电子态密度、能带结构、介电函数、吸收系数和折射率等电子结构及光学特性参量。计算结果表明：该类晶体的价带和导带部分重合，具有典型半金属特性，其费米面附近的态密度主要是由Mo或W原子中的d电子和Si原子3p态杂化而成，对晶体导电性贡献最大的是Mo和W原子中的d电子，其光学性质表现出各向异性，沿*c*轴方向介电函数和折射率都存在1个向低能方向偏移(红移)且峰值较大的峰；具有$C11_b$型结构的$MoSi_2$和$WSi_2$由于Mo和W原子价电子不同导致其电子结构和光学性质存在微小差别。

关键字：平面波赝势方法；电子结构；光学性质

# Numerical investigation on electronic structures and optical properties of $MoSi_2$ and $WSi_2$ single crystals

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**Abstract:**The electronic structures and optical properties of $MoSi_2$ and $WSi_2$ single crystals with the $C11_b$ structure were computed by using the plane pseudo-potential method based on the density functional theory. The generalized-gradient approximate (GGA) was used for the exchange-correlation potential. The calculation result shows that those $MoSi_2$ and $WSi_2$ single crystals are of characteristics of a half-metal owing to the partial overlaps of the valence and conduction-band and it is d electrons in atom Mo or W that play a main role in the electrical conductivity. For the optical properties, the anisotropic of these models is proved by simulation results and the dielectric function, the absorption spectra and the refractive index present different behaviors for polarized light in different directions. In addition, while having the similar properties, the electronic structures and optical properties have subtle differences between $MoSi_2$ and $WSi_2$ because of the difference in the structure.

**Key words:**plane pseudo-potential method; electronic structure; optical property

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