Insight into the oxidation mechanism of $MoSi_2$: Ab-initio calculations

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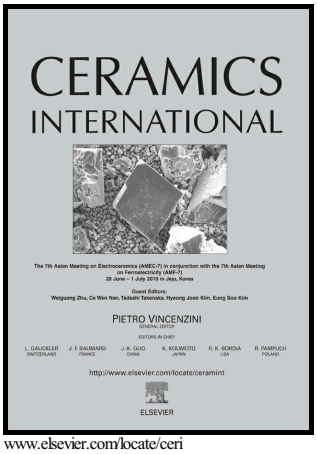

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Insight into the oxidation mechanism of $MoSi_2$: Ab-initio calculations

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Abstract:

Transition metal silicides (TMSis) are potential candidates for high-temperature applications. However, the improvement of oxidation resistance of TMSis is still a big challenge due to the formation of volatile oxides. To overcome the important problem, we use the *ab-initio* calculations to study the oxidation mechanism of $MoSi_2$ and investigate the influence of Al and Cr on the oxidation resistance of $MoSi_2$. Two possible O-doped sites: octahedral interstitial site and tetrahedral interstitial site are considered. We find that oxygen prefers to occupy the TI-2 site because of the strong charge interaction between Si and O. We further examine the alloying effect in $MoSi_2$. Cr-doping is a thermodynamically stable in contrary to Al-doping is a thermodynamically instable. Importantly, alloying elements can effectively improve the oxidation resistance of $MoSi_2$ because those alloying elements enhance the localized hybridization between Si and O. Finally, our work can open up a new path to improve the