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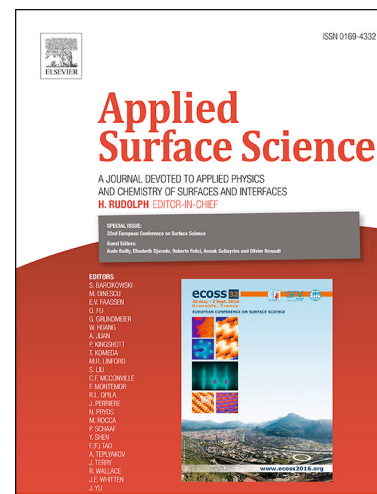
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Li decorated Be₃C₂ as light-weight host material for reversible hydrogen storage

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Abstract

Deficiency of appropriate host materials with high gravimetric density for hydrogen storage impedes the development of hydrogen economy and its downstream application, *i.e.*, hydrogen fuel battery. Within the framework of density functional theory, we investigate systematically the performance of Li decorated Be₃C₂ for hydrogen adsorption and reversible storage. We find that Li atoms forms strong bond with the light-weight Be₃C₂ substrate without the issue of agglomeration, where dispersive decoration of Li on Be₃C₂ is calculated to be more energetically than Li metallic clusters. As for Li doped Be₃C₂ system, a maximum gravimetric hydrogen density of 10.79 wt% could be reached. Such high-capacity benefits from the light-weight of the host and its strong binding to H₂ molecules, in which both polarization and electronic hybridization mechanism play a significant role. Hydrogen storage under different pressure and temperature has also been discussed based on thermodynamic analysis and a practical capacity of 9.27 wt% could be expected under more realistic operation of hydrogen fuel battery (stored at 30 atm/25 °C and released at 3 atm/100 °C). Favorable hydrogen adsorption capability and desired storage/release dynamic performance endows Li decorated Be₃C₂ with promising applications in hydrogen energy storage field.

Key words: Hydrogen host material, Be₃C₂, Lithium decoration, First-principle

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