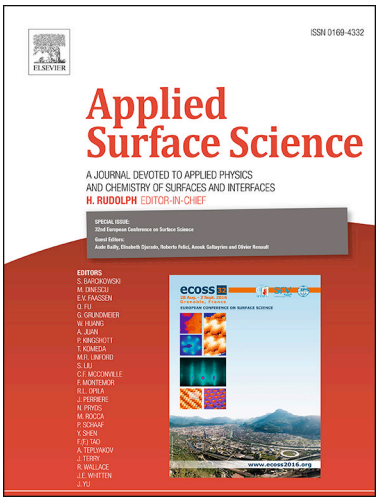
# Accepted Manuscript




Full Length Article

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# Li decorated $Be_3C_2$ 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 $Be_3C_2$ for hydrogen adsorption and reversible storage. We find that Li atoms forms strong bond with the light-weight $Be_3C_2$ substrate without the issue of agglomeration, where dispersive decoration of Li on $Be_3C_2$ is calculated to be more energetically than Li metallic clusters. As for Li doped $Be_3C_2$ 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 $H_2$ 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 ℃ and released at 3 atm/100 ℃). Favorable hydrogen adsorption capability and desired storage/release dynamic performance endows Li decorated $Be_3C_2$ with promising applications in hydrogen energy storage field.

**Key words**: Hydrogen host material, $Be_3C_2$, Lithium decoration, First-principle

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