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Clarifying the capacity deterioration mechanism sheds light on the design of ultra-long-life hydrogen storage alloys

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ABSTRACT

The intrinsic relationship between the atomic structure and macroscopic corrosion behavior has been established, which proposes that the atomic coordination state is another key factor affecting the corrosion resistance and cycling life of hydrogen storage alloys besides elements electronegativity. The density functional theory simulation and experimental results confirm the predictions, shedding light on the design of ultra-long-life hydrogen storage alloys. The as-designed alloy $La_{0.73}Ce_{0.17}Y_{0.1}Ni_{3.75}Co_{1.0}Mn_{0.3}Al_{0.35}$ exhibits an ultra-long 2415-cycle life, which is almost five times that of the traditional commercial alloy. The usage costs of nickel metal hydride battery based on this alloy is only 1/5 that of Li-ion battery, showing broad market prospect.

Keywords: Hydrogen storage alloy; Nickel metal hydride battery; Cycling life; New-energy vehicle, Surface coordination state

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