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Structural, Electronic, and Hydriding Properties of Li_2MgSi JAN HERBST, MARTIN MEYER, GM R&D Center — An investigation of Li_2MgSi, with particular emphasis on its potential as a hydrogen storage material, is reported. A cubic $P\bar{4}3m$ crystal structure, differing from previous determinations, is established. We find that the material reversibly sorbs ∼2.8 mass% hydrogen at T ∼ 300 °C according to the reaction $Li_2MgSi + H_2 \leftrightarrow \frac{1}{2}Mg_2Si + 2LiH + \frac{1}{2}Si$. Electronic structure calculations indicate that Li_2MgSi is a semiconductor with a small, indirect gap of ∼0.2 eV.

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