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Synthesis of Li_2MgIr and $LiMgIrH_6$: Guidance from DFT JAN HERBST, JAMES SALVADOR, MARTIN MEYER, GM R&D Center — Formation of Li_2MgIr was suggested by theoretical modeling of Li_2MgX systems and their hydrides with density functional theory (DFT). Verifying our DFT results, we have synthesized Li_2MgIr and determined its crystal structure and hydrogen sorption behavior. The phase crystallizes in the cubic $P\bar{4}3m$ space group and is isostructural to the known ternary Li_2MgSi. Its reaction with hydrogen proceeds according to $Li_2MgIr + \frac{7}{2}H_2 \rightarrow LiMgIrH_6 + LiH$. The hydride $LiMgIrH_6$ also features $P\bar{4}3m$ symmetry; its detailed crystal structure is established via a combination of x-ray diffraction and DFT analyses. A metal $\rightarrow$ insulator transition accompanies formation of the hydride.

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