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**Fullerene mediated hydrogen release in lithium borohydride** RALPH SCHEICHER, Uppsala University, SA LI, PURU JENA, Virginia Commonwealth University, UPPSALA UNIVERSITY COLLABORATION, VIRGINIA COMMONWEALTH UNIVERSITY COLLABORATION — Complex metal hydrides possess many properties which make them attractive as a storage medium for hydrogen, but typically, catalysts are required to lower the hydrogen desorption temperature and to facilitate hydrogen uptake in the form of a reversible reaction. The overwhelming focus in the search for catalyzing agents has been on compounds containing titanium, but the precise mechanism of their actions remains somewhat obscure. A recent experiment has now shown that fullerene (C60) can also act as catalysts for the hydrogen uptake and release in lithium borohydride ($LiBH_4$). In an effort to understand the involved mechanism, we have employed density functional theory to carry out a detailed study of the interaction between this complex metal hydride and the carbon nanomaterial. Considering a step-wise reduction of the hydrogen content in $LiBH_4$, we find that the presence of C60 can lead to a substantial reduction of the involved H-removal energies. This catalyzing effect is explained by us as a consequence of the interaction between the $BH_x^-$ part and the C60 entity.

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