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Quasi-Elastic Neutron Scattering Studies on Solid Electrolytes for solid-state Lithium Batteries

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The development of better batteries is paramount for the spread of renewable electricity production and utilisation. Limited improvement are expected for lithium-ion battery, because of the use of organic liquid electrolytes. An alternative is to use solid electrolyte instead.
The high temperature (> 383 K) phase of lithium-borohydride, is a fast Li+ conductor. The fast conduction is kept at room temperature by stabilizing the phase via solid solution with Li-halides or confinement of LiBH4 in nanoporous scaffolds.
We have studied, in LiBH4:LiI, the Li+ diffusion using QENS and DFT. Lithium defects are easily formed at room temperature and low energy barriers were found between stable defect sites, favoring high defect mobility (Fig.1-a).
QENS was also used to probe the dynamic of the BH4– anions in LiBH4 confined in nanoporous SiO2. Four quasi-elastic components were found in two different temperature domains. (Fig.1-b). The narrow components, at high temperature, are associated with reorienting BH4– in crystalline LiBH4, while the broader components at low temperature, with much more rapidly reorienting BH4–, can be associated with the LiBH4 located at the SiO2 surfaces, suggesting that the high conductivity occurs at the interface between LiBH4 and SiO2.

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