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2014-53/50 Halogen-Free Electrolytes

Currently used electrolytes ...

... in Li-ion batteries mostly contain toxic halogens. In their Communication on page 13916, P. Jena et al. use first-principles calculations to show that all these electrolytes are based on superhalogens, i.e., that the vertical electron detachment energies of the moieties that constitute the anions are larger than those of any halogen atom. Several superhalogens do not contain a single halogen atom and their potential as effective electrolytes was studied. Among the identified halogen-free electrolytes, $\text{Li}(\text{CB}_{11}\text{H}_{12})$ is shown to have the greatest potential.

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