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Vacancy-mediated electrical conductivity in lithium fluoride upon moderate heating

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The challenge posed by charge accumulation at the interfaces of low dimensional electronic devices has resulted in a wide range of novel architectures as well as potential applications in organic electronics such as organic photovoltaics. These devices include, among others, organic light-emitting diodes and organic thin-film transistors. Within such devices, the use of lithium fluoride (LiF) as an inter-facial layer reduces the potential barrier at the interface which facilitates the efficient collection of photo-generated charge with minimal energy 1. This manifests itself in minimising the band bending at interfaces of such devices and is attributed to the low work function of LiF, which reduces the effective work function at the interface [2] and in turn leads to efficient charge extraction/injection in the organic layer [3]. Thus the electrical properties of LiF are a subject of interest. While most alkali halides have been extensively investigated, LiF is an exception which, to date, has not been given enough attention. We show that lithium fluoride conducts electricity on heating to temperatures well below its melting point. By examining the variation in conductivity with heating along (111) plane, we show that the conductivity is due to a mechanism of ion hopping and vacancy migration through the host lattice sites. By fitting the data into the Nernst-Einstein relation the two linear regions were obtained from which upon extrapolation the activation energies for ion hopping were found to be 0.67 eV and 0.35 eV for high-temperature (region I) and low-temperature (region II) regions respectively as shown in the figure below. Conductivity of LiF has implications for its use as an inter-facial layer in photovoltaic device design and potential use in bio-sensing devices due to its cell tissue effective mass equivalence.

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