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Simultaneous enhancement of electronic and Li+ ion conductivity in LiFePO4[1] JAEKWANG LEE, Oak Ridge National Laboratory and Vanderbilt University, STEPHEN J. PENNYCOOK, Oak Ridge National Laboratory, SOKRATES T. PANTELIDES, Vanderbilt University — The electronic conductivity is generally highly sensitive to the electronic properties of a material while the ionic conductivity is mainly sensitive to the structural properties. Thus, the simultaneous control of both is very challenging. Furthermore, many electrochemical systems for advanced energy technologies require materials in which both ionic and electronic conductivities are optimized. Here we explore the influence of biaxial strain on the electronic and Li^+ ion conductivities of the battery cathode material $LiFePO_4$ by performing first-principles calculations. We show that biaxial tensile strain leads to simultaneous increases in electronic and ionic conductivities of $LiFePO_4$. The results unveil a generic mechanism that should be present in other materials with polaronic transport and provide a promising new approach to enhance the performance of energy-related materials.

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