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Prof. Francesco Ciucci is an associate professor at the Hong Kong University of Science and Technology. He graduated *cum laude* from Politecnico di Milano, Italy and Ecole Centrale de Paris, France with degrees in Aerospace Engineering and Applied Physics, respectively. He pursued his PhD in Engineering from the California Institute of Technology, USA, where he was supported by the internationally renowned Rotary Ambassadorial Scholarship (he was one of the three Italian recipients receiving this award in 2002). Francesco did his postdoctoral work at the Heidelberg Graduate School of Mathematical and Computational Methods for the Sciences of the University of Heidelberg, Germany. There, he obtained a Marie Curie Fellowship and a Heidelberg Graduate School Fellowship. His research articles have been featured in major journals, including, Nature Chemistry, Advanced Energy Materials, Chemistry of Materials, Chemical Reviews and many more. Francesco's current research centers around solid-state energy materials, including those used in fuel cells and solid-state batteries, with particular emphasis on the modeling of such systems and the development of new ceramic materials.

Ionic Materials for Energy Storage and Conversion

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In this presentation, I will discuss my group's ongoing activities in the area of ionic materials for solid-state batteries and solid oxide fuel cells. In particular, I will discuss our ongoing research in the area of atomic simulations for electrolyte materials as well our experimental work on ceramic Li electrolytes.

I will first give specific examples regarding, lithium-rich anti-perovskites (LiRAPs) a promising family of solid electrolytes, which exhibit ionic conductivities above 10^{-3} S cm^{-1} at room temperature, among the highest reported values to date. I will discuss the chemistry and the associated lithium transport in Li_3OCl, a prototypical LiRAP, using DFT calculations and classical MD simulations. We studied three types of charge neutral defect pairs, namely the LiCl Schottky pair, the Li_2O Schottky pair, and the Li interstitial with a substitutional defect of O on the Cl site. Among them the LiCl Schottky pair has the lowest binding energy and is the most energetically favorable for diffusion as computed by DFT. This is confirmed by classical MD simulations, where the computed Li ion diffusion coefficients for LiCl Schottky systems are significantly higher than those for the other two defects considered and the activation energy in LiCl deficient Li_3OCl is comparable to experimental values. The high conductivities and low activation energies of LiCl Schottky systems are explained by the low energy pathways of Li between the Cl vacancies. We propose that Li vacancy hopping is the main diffusion mechanism in highly conductive Li_3OCl.

I will then discuss the structural origin of the superionic conductivity in Li and Na conductivity on closo-borates, linking these properties to structure. I will also overview the link between structure and conductivity in Li-stuffed garnets using data-mining.

I will conclude with an overview my group's ongoing effort in the area of solid-state batteries.