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Determination of Raman Spectrum of $\text{Li}_{28}\text{La}_{12}\text{Zr}_8\text{O}_{48}$ as a Function of Dopant SAIKAT MUKHOPADHYAY, Cornell Nanoscale Facility, Cornell University, Ithaca, NY, TRAVIS THOMPSON, JEFF SAKAMOTO, Department of Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI, MICHELLE JOHANNES, Naval Research Laboratory, Washington, DC, DEREK STEWART, Cornell Nanoscale Facility, Cornell University, Ithaca, NY — $\text{Li}_{28}\text{La}_{12}\text{Zr}_8\text{O}_{48}$ is a supervalent conductor with a low conductivity tetragonal phase and a high conductivity cubic phase, making it a strong candidate as a practical Li ion rechargeable battery solid electrolyte. The high conductivity phase can be stabilized via supervalent doping that drives Li^+ ions out of the lattice, creating vacancies that both relieve the necessity for Li sublattice ordering and provide easier pathways for ionic conduction. The conductivity strongly depends on both doping concentration and site preference. Ta^{5+} has been suggested as an optimal dopant as it likely substitutes for Zr^{4+} , thereby leaving the Li sublattice undisturbed. However, it is difficult to accurately establish the actual, as compared to nominal, amount of Ta doped into the lattice which, in turn, determines the vacancy concentration and conductivity. In this talk, we will present the variation of Raman intensities of LLZO as a function of Ta concentration to determine the role of dopant and vacancies in deciding measured Raman intensities via first principles calculations based on Density Functional Theory. A direct comparison of calculated and measured Raman spectrum may provide a definitive measure of vacancy concentration.

Saikat Mukhopadhyay
Cornell Nanoscale Facility, Cornell University, Ithaca, NY

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