Presentation title: Computationally predicted highest Li-superionic conductor electrolyte for solid state battery.

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Presentation type: Oral presentation

Abstract (250-300 words):

Solid-state batteries are a promising alternative to conventional Li-ion batteries, as they offer higher safety, durability, and performance. However, their efficiency depends on the development of solid electrolytes that enable fast and stable Li-ion transport across the electrodes. Among various electrolyte candidates from the polysulfide, oxide, argyrodite, and perovskite families, Li_6PS_5Cl stands out due to its superionic conductivity of lithium at room temperature and broad electrochemical stability window. Based on our computational study, we have recently discovered a new composition from the polysulfide family, $Li_5PS_4Cl_2$, which exhibits highest solid-state Li-ionic conductivity at room temperature, approximately 20 mS/cm. We used molecular dynamics simulations to reveal the underlying mechanisms of Li-ion diffusion in these materials and to evaluate their compatibility with S-based cathodes. We find that Li-ion migration is governed by a cooperative substitutional mechanism that involves multiple Li-ions and Li-vacancies in a 3D network. We also show that the Li-ion conductivity and the activation energy are consistent with experimental NMR measurements. Furthermore, we demonstrate that the solid electrolytes are thermodynamically stable with the S-based cathodes and can reproduce the experimental discharge curves using reactive molecular dynamics (RMD). We studied the interfacial stability of the solid electrolyte with an S-based cathode and Li-anode using RMD. Reax force field parameters were developed using DFT studies on small molecular systems. The discharge process was simulated by incrementally adding Li to the fully charged state (Li_3PS_9), and the discharged structure was obtained ($Li_{12}PS_9$) and was well compared with the experimental discharge curve, as shown in our recent publication. Our results provide valuable insights into the design and optimization of solid-state batteries based on Li-superionic conductors.

Biography (150-200 words):

Tridip Das is a staff scientist at California Institute of Technology, working on quantum mechanics, molecular dynamics, and other fields. He is passionate about solving problems in energy and materials science using computational tools and data-driven approaches. He has made significant contribution in the area of solid-state battery research. He is also involved in diverse research area including polymer upcycling, CO2RR, NH3 synthesis, heterogeneous catalysis. He received his Ph.D.

in Chemical Engineering and Material Sciences from Michigan State University in 2017. His PhD research focused on oxygen vacancy formation and transport in solid oxide fuel cell components. He got his M. Tech. and a B. E. in Chemical Engineering from India.