Defects, graphs and route-finding:

Probing ion transport using time-based centrality

Konrad S. Gomez-Haibach[1, 2], Maria A. Gomez*[2], Andrew Carl Grieder[3] and Nicole Adelstein[4]

[1]WPI, [2]Mount Holyoke College, [3]University of California Santa Cruz, and [4] San Francisco State

Using the inverse of the average time to first return to the initial site as a centrality measure, we assessed ion conduction in the presence of other conducting ions. High centrality locations have short return times. Short return times occur when the ion is either on a fast path which travels periodically through the system, a highway, or the ion only travels through nearby sites and returns quickly, a trap region. Centrality measure images allow us to see both ion traps and highway paths through the system at once. These high centrality sites appear dark in our model. Considering the removal of vertices from the original connected graph when they are occupied by other ions (top image), we calculated the fundamental matrix centrality shortened by the removal of rows and columns corresponding to the removed vertices. The centrality image showed that a second proton moves close to the first proton in yttrium doped barium zirconate as seen in the bottom left image. In amorphous LLZO ($Li_7La_3Zr_2O_{12}$), centrality highlights remaining long pathways, which are taken by kinetic Monte Carlo as seen in the bottom right image. However, the noise in graph parameters can significantly distort the resulting centrality image. Despite this, centrality measures seem to be useful even with the removal of vertices or possible sites for the conductor.