

- Objective:

- » Calculate and visualize Brillouin zones of atomic structures

- Approach:

- » Employ QHULL to calculate Voronoi cell of reciprocal lattice
- » Save to VTK file (PolyData format) for visualization

- Results / Impact:

- » Separate “Simulation” provides ability to visualize any atomic structure
- » All lattice types possible (diamond, zincblende, wurtzite, rhombohedral)
- » New nanoHUB tool under development (w/ Arun Goud, Purdue)

