MECHANISTIC INSIGHTS INTO HYDRATION OF SOLID OXIDES

Research Challenge
• Solid oxide electrolysis cells (SOEC) operating at a high temperature will help reduce cost and enhance efficiency for hydrogen production as an alternative energy source.
• SOECs with proton-conducting electrolytes such as Y-doped SrZrO3 (SZY) can produce pure and dry hydrogen.
• The design and development of solid oxide electrolytes with sufficient stability and enhanced conductivity for SOEC are still a challenge.

Methods & Codes
• Density functional theory (DFT) calculations are used to investigate the hydration behavior of solid oxides and performed using the Vienna Ab initio Simulation Package (VASP)
• The cutoff energy for the plane-wave basis set was 500 eV for all calculations. All the calculations are spin polarized. Bader population analysis is performed to calculate the atomic charges.

Results & Impact
• The project investigated the hydration processes in two solid oxides with a single-crystal structure—a proton-conducting SZY and an oxide ion-conducting YSZ.
• Results - both the SrO (001) surface of SZY and (111) surface of YSZ are favorable for the adsorption of water. The structural minimization and charge analyses indicate that the water molecule is adsorbed as two hydroxide ions on the surface improving the efficiency of the process

Why Blue Waters
• Large-scale ab initio simulations are needed to obtain the dynamics of hydration in solid oxides.
• For these calculations, using multiple nodes for each job achieves the best performance and the highest productivity of the science team.
• The computational productivity improvement is attributed to the power of Blue Waters and the support of project staff.