Mechanistic insights into hydration of solid oxides

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Abstract

Compared to a commercially available polymer electrolyte membrane (PEM) based low temperature electrolysis cell, a solid oxide electrolysis cell (SOEC) operating at a high temperature can take advantage of thermal energy to reduce electrical energy demand resulting in a reduced cost and enhanced efficiency for hydrogen production. Some solid oxide materials, used in solid oxide fuel and electrolysis cells, are known to conduct protons once they are hydrated. However, the mechanisms by which solid oxide materials get hydrated is not clear.

In this seminar, the mechanistic insights into hydration of solid oxides will be introduced. Density functional theory (DFT) calculations are performed to investigate hydration of two typical solid oxides – a proton conducting yttrium-doped strontium zirconate (SZY) and an oxide ion conducting yttria-stabilized zirconia (YSZ). We suggest a four step process to understand hydration of solid oxides – water adsorption on the surface, proton migration from the surface to bulk, proton migration in the bulk, and oxide ion vacancy migration in the bulk. Our results indicate that the primary difference between the hydration of SZY and YSZ comes from the energy barriers for proton migration from the surface to the bulk of the oxide material. In addition, the mechanism of OH transport between surface and subsurface in the perovskite is proposed. The current results not only provide mechanistic insights into the hydration of SZY and YSZ, but also the importance of structural rearrangements when a proton is incorporated into the bulk of the solid oxide material.

About the Speaker

Dr. Jing received his BS at Wuhan University in 2004, and MS and PhD at Harbin Institute of Technology (HIT) in 2007 and 2011, respectively, in China. During the time from 2009 to 2011, he studied at University of Illinois at Urbana-Champaign (UIUC) as a Joint PhD student. He joined the faculty as a lecturer at HIT in 2011. From 2015, he became a associate professor in HIT. At the same time, he went back to UIUC as a postdoctoral researcher, and joint a renewable energy project led by Illinois and Kyushu researchers, this research is funded by the Partnerships for International Research and Education (PIRE) program. Regarding to requirement of PIRE program, he will work in Professor Matsumoto's laboratory for two months and participate in research activities and exchanges with research collaborators at International Institute for Carbon-Neutral Energy Research (WPI-I2CNER) at Kyushu University. His research focuses on dynamic properties of hydration in solid oxides, Nanomechanics, Heat transfer, Force field development. Computational methods involves molecular dynamics (MD), Density functional theory (DFT), and multiscale methods. He published about 30 international journal papers.