Materials Design from Advanced Optimization and High-throughput Screening

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Nowadays, researchers have applied various optimization techniques to develop new materials with targeted properties by manipulating the design variables such as chemistry, structure, thermodynamics and operation conditions. Among them, material's structure prediction is a classical optimization challenge that aims to find the lowest-energy atomic model for a given chemical input. Recent breakthroughs in structure prediction in conjunction with accurate quantum mechanic calculation have allowed the structures of many new and increasingly complex materials to be anticipated. In this talk, I will first demonstrate the power of structure prediction by reviewing several example studies on both inorganic and organic functional materials. Furthermore, I will introduce the ongoing software development efforts in my group to address the challenge of autonomous computational materials discovery by coupling materials structure prediction with group theory, machine learning and high-throughput screening techniques. Some preliminary screening results on energy and electronic materials will be discussed as well.

Short bio: Qiang Zhu received the Ph.D. in Mineral Physics from Stony Brook University in 2013, as well as a B.S. in Materials Science from Beihang University of China in 2007. In 2016, he joined the University of Nevada Las Vegas (UNLV) as an Assistant Professor in Physics. At UNLV, he is leading a research group in computational physics and materials discovery. He has published over 70 papers in the peer reviewed journals including 1 Science, 1 Nature Chemistry, 1 Nature Rev. Mater., 3 Nature Communication, 5 PRL, 1 JACS, 2 Angew. Chem., and 2 Matter. He is also the recipient of the President's award for distinguished Doctoral Students at Stony Brook University (2013), the NSF CAREER award (2021), and the DOE CAREER award (2021).