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Wai-Yim Ching

University of Missouri-Kansas City, USA

Abnormal deformation behavior in a super-soft material: Amorphous zeolite imidazolate framework (a-ZIF)

Metal-organic frameworks (MOFs) materials have attracted immense attention from diverse disciplines of chemistry, physics, engineering, material sciences, biological and biomedical sciences. Zeolitic imidazolate framework (ZIF) is an important member of MOF with network topologies analogous to silica. In the network, the corner-sharing SiO_4 tetrahedra are replaced by MN_4 tetrahedra (M=metal, Zn in this work) linked by imidazolate (IM) $(C_3N_2H_3)^-$anions. The chemically tunable porosities of ZIFs are pivotal for many of their potential application. There exist a large number of crystalline ZIFs with well-defined zeolite structures; the emerging category of non-crystalline or amorphous ZIF (a-ZIF) is of particular interest. The a-ZIF can be viewed as a model system for understanding the general features and properties of a novel hybrid inorganic/organic glass with no long range order (LRO) but with well-preserved short range order (SRO). We have recently constructed a large a-ZIF mode and studied its electronic structure, inter-atomic bonding and optical properties. In this talk, I present further study of the deformation behavior of this interesting material by applying step-wise homogenous compression and extension with strains respectively up to -0.30 and +0.30. The data for stress vs. strain at each step are fully analyzed including mechanical properties. It shows that a-ZIF is a super-soft material with intricate properties that have not been seen before. The origin of this behavior is explained by detailed electronic structure and bonding investigation. Our investigation shows that a-ZIF belongs to a class of super-soft materials with some intricate properties previously unknown. Additional large-scale accurate simulations may reveal other properties for potential applications especially in the soft covalent organic framework (COF) materials.

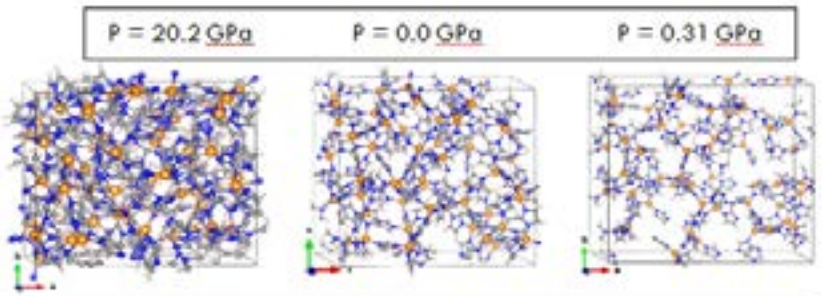

Figure 1: Ball and Stick figure of a-ZIF model at high compression (left), zero strain (middle) and high extension (right).

Biography

Wai-Yim Ching is a Professor of Physics at University Missouri-Kansas City, USA. He leads the Electronic Structure Group (ESG) in the Department of Physics and Astronomy. His research focuses on condensed matter theory and computational materials science using first-principles methods. With more than 40 years of experience, he is an author or co-author of over 410 articles in diverse areas related to materials. He is an Academician of World Ceramic Academy, a Fellow of the American Ceramic Society and the American Physical Society. He is an Associate Editor of *Journal of the American Ceramic Society*.

chingw@umkc.edu