"Computational Design of Mechanically Flexible Organics"

Physical Chemistry Seminar

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10:30-11:30a.m. BRWN 4102

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Abstract:

Recently, some organic crystals have been found to be surprisingly flexible by undergoing a large extent of elastic or plastic deformation upon mechanical loads. Despite the increasing experimental reports on such mechanically flexible crystals, this phenomenon has never been reproduced in numerical simulation and thus there is no atomistic mechanism to explain its physical origin. Using three recently reported naphthalene diimide derivatives as the examples, we performed the first direct molecular dynamics simulation to model their mechanical behaviors from brittle fracture to elastic/plastic deformation upon mechanical bending. Our simulation reveals that molecular rotational freedom is the key factor to determine the crystal's mechanical response. Furthermore, we propose to use spherical harmonic transform and first-principles crystal structure prediction to screen and design new mechanically flexible candidates with better functionalities. The combination of different computational techniques is promising to harvest new bendable organics for future technological applications.

Bio: Qiang Zhu is currently an associate professor in Mechanical Engineering at the University of North Carolina at Charlotte (UNCC). He received the Ph.D. in Mineral Physics from Stony Brook University in 2013, as well as a B.S. in Materials Science and Engineering from Beihang University of China in 2007. Between 2016-2023, he was a faculty member in Physics at the University of Nevada Las Vegas (UNLV). His group has launched several open-source projects in high throughput materials simulation and machine learning, as well as materials discovery. He has published over 80 papers in peer reviewed journals. He is also the recipient of the President's award for distinguished Doctoral Students at Stony Brook University (2013), the NSF CAREER award (2021), the DOE CAREER award (2021), and the Barrick Scholar Award (2022).

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