Contribution ID: **54** Type: **Talk**

Computational material synthesis: Atomistic and molecular dynamics, and bio-inspired AI (30 min talk + 15 min discussion)

Wednesday, 14 April 2021 13:45 (45 minutes)

Nature produces a variety of materials with many functions, often out of simple and abundant materials, and at low energy. Such systems - examples of which include silk, bone, nacre or diatoms - provide broad inspiration for engineering. Here we explore the translation of biological composites to engineering applications, using a variety of tools including molecular modeling, AI and machine learning, and experimental synthesis and characterization. We review a series of studies focused on the mechanical behavior of materials, especially fracture, and how these phenomena can be modeled using a combination of molecular dynamics and machine learning. We also present various case studies of hierarchical material optimization using genetic algorithms, applied to 3D printed composites, protein design, and a translation of protein folding to music and back, to offer a broad bio-inspired AI-driven material synthesis platform. As an example we present a recent study in which we translated JS Bach's Goldberg Variations into protein form, and elucidated salient features of the resulting molecular conformations and material functions.

Poster title

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