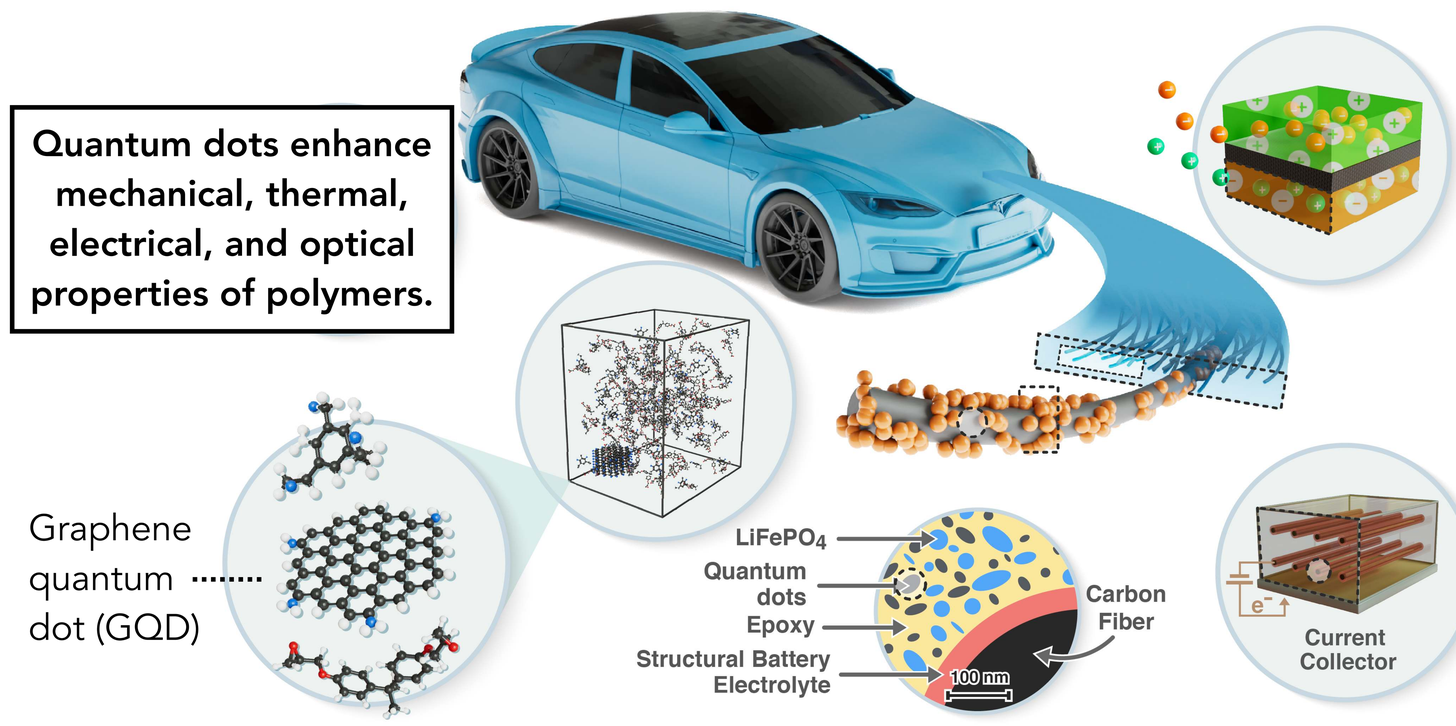
Multi-Scale Mechanical Behavior of Quantum Dot Nanocomposites: Towards Data-Driven Automatic Discovery of High-Performance Structures

Özgür Keleş and Swapnil Bamane
Department of Mechanical Engineering and Engineering Science
University of North Carolina at Charlotte, NC 28223

UNIVERSITY OF NORTH CAROLINA CHARLOTTE

Abstract: Brittle epoxy matrices often serve as the principal failure point in composites. Matrix enhancements can be achieved by optimizing polymer blends to maximize intermolecular interactions or by introducing fillers. While nanofillers such as clay, rubber, carbon nanotubes, and nanoplatelets enhance mechanical properties, they can lead to issues like agglomeration, voids, and poor load transfer. Quantum dots, being the smallest nanofillers, offer higher dispersion and the potential to promote intermolecular interactions, enhancing **stiffness, strength, and toughness** simultaneously. This study employed molecular dynamics simulations to design graphene quantum dot (GQD) reinforced epoxy nanocomposites. By functionalizing GQDs with oxygen-based groups—hydroxyl, epoxide, carboxyl, and mixed chemistries—their effects on the mechanical properties of nanocomposites were systematically evaluated. Results show that hydroxyl-functionalized GQDs provide optimal performance, increasing stiffness and yield strength by 18.4 and 56.1%, respectively. Structural analysis reveals that these GQDs promote a closely packed molecular configuration, resulting in reduced free volume. The effects of quantum dot vol. % on the mechanical behavior was also investigated together with thermal properties, where the curing shrinkage reduced by 20%.

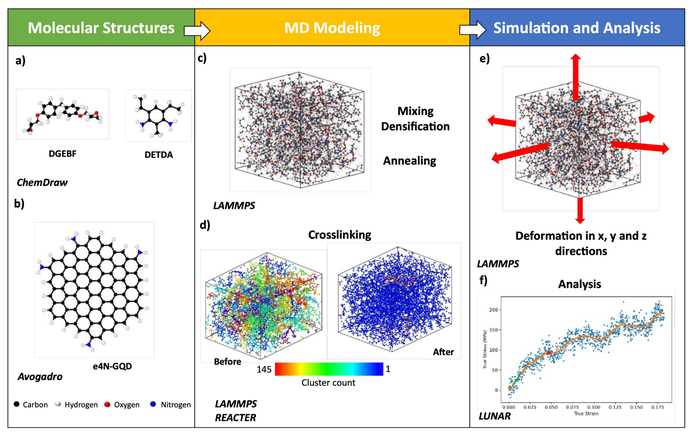
Quantum Dot Structural Nanocomposite Batteries

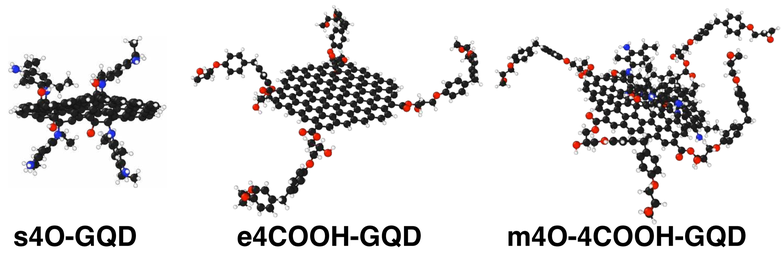


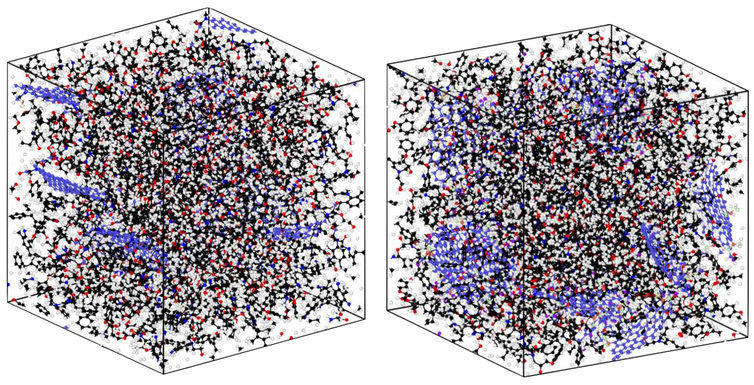
How?

↓

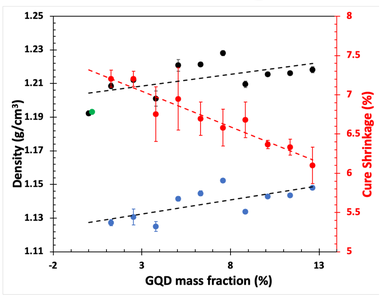
Molecular dynamics simulations of quantum dot nanocomposites



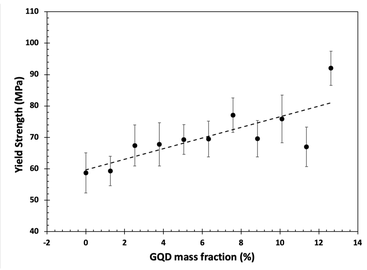




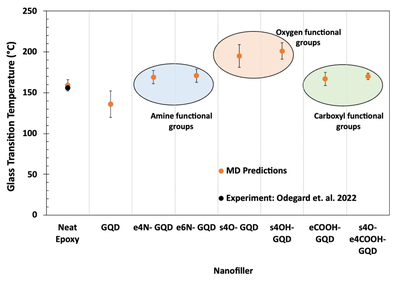
20 % reduction in shrinkage



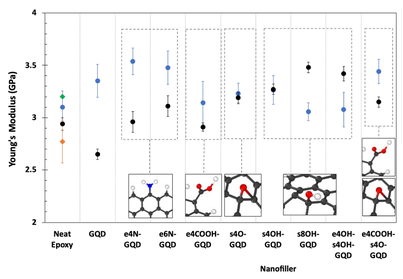
50 % increase in yield strength



30 % increase in Tg

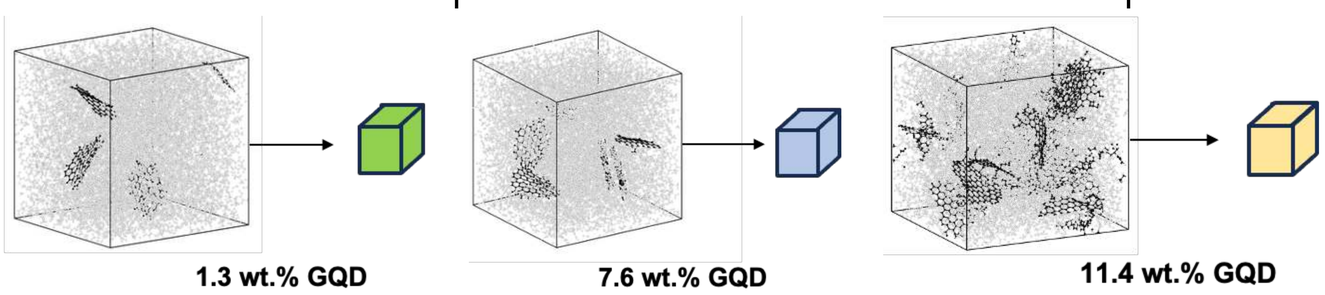


20 % increase in stiffness



Mechanics of multi-scale quantum dot-carbon fiber composites

Nano-scale

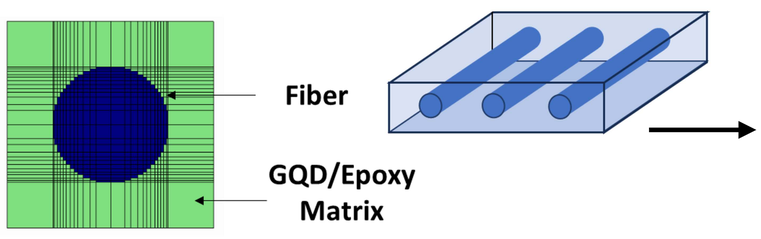


↓

Micro-scale

↓

Macro-scale



CF/GQD/Epoxy Hybrid RUC

This research was funded by U.S. National Science Foundation CAREER award, grant #2450841. Special thanks to Dr. Nakhiah Goulbourne and Dr. Siddiq Qidwai—**NSF MOMS**.

References

1. Keleş, Özgür, and Prathamesh P. Deshpande. "Mechanical behavior of graphene quantum dot epoxy nanocomposites: A molecular dynamics study." *Materials Letters* 362 (2024): 136206.
2. Deshpande, Prathamesh P., et al. "Optimizing Epoxy Nanocomposites with Oxidized Graphene Quantum Dots for Superior Mechanical Performance: A Molecular Dynamics Approach." *ACS omega* 10.14 (2025): 14209-14220.
3. Bamane, Swapnil S., and Ozgur Keles. "Effects of Graphene Quantum Dots on Thermal Properties of Epoxy Using Molecular Dynamics." *Applied Nano* 6.3 (2025): 15.
4. Deshpande, Prathamesh, Robert Chan-Jobe, and Ozgur Keles. "Molecular structure data and modelling roadmap for optimized oxidized graphene quantum dot and epoxy interface and mechanical properties." *Data in Brief* 57 (2024): 111059.
5. Deshpande, Prathamesh P., and Ozgur Keles. "Simulation data for engineering graphene quantum dot epoxy nanocomposites using molecular dynamics." *Data in Brief* 53 (2024): 110169.
6. Kemppainen, Josh, et al. "LUNAR: automated input generation and analysis for reactive LAMMPS simulations." *Journal of chemical information and modeling* 64.13 (2024): 5108-5126.