



CMCC Mechanochemistry Discussions

Online Seminar Series

High-Throughput Discovery of Ferrocene Mechanophores with Enhanced Reactivity and Network Toughening

Livestreaming at
11:15 AM (CT)
THURS., March 19, 2026

on the CMCC YouTube Channel:

<https://www.youtube.com/channel/UC7eCYPKbGTKpgO7W2bNABxg>



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Mechanophores (i.e., force-responsive molecules embedded in materials) have opened new opportunities in chemical reactivity and materials design. Nevertheless, the accessible design space, especially of transition metal mechanophores, remains largely unexplored. Ferrocene is an especially promising mechanophore scaffold due to its high thermal stability and mechanochemical lability, but only a few examples of ferrocene-derived mechanophores had been realized compared to the thousands of known ferrocene complexes. I will present our computational and machine learning-guided discovery of synthesizable ferrocene mechanophores. Through data-driven screening of 12,000 candidate materials, we uncovered design principles that tune mechanochemical activation, including steric transition-state stabilization and non-covalent ligand interactions that alter reaction pathways. Experimental validation at both the polymer strand and network levels confirms our predictions, with a computationally discovered ferrocene cross-linker producing more than a fourfold increase in material tearing energy.



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