



CMCC Mechanochemistry Discussions

Online Seminar Series

Forces That Shape Chemistry: Mechanochemical Pathways to Direct Bond Formation in Solids

Livestreaming at
10:00 AM (CT)
THURS., February 19, 2026

on the CMCC YouTube Channel:

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



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Solid-state materials are governed by the interplay of chemical bonding, connectivity, and composition, and their reactivity can be dramatically altered by applying mechanical stress. In this talk, I will show how electronic structure calculations based on density functional theory (DFT) reveal how specific stress states reshape these “3Cs” to enable chemical transformations not accessible in solution. Using the compound HgNCN as a model system, we show that hydrostatic pressure can convert the cyanamide form of the NCN anion into the carbodiimide form across an isosymetric structural transition. This force-driven pathway mirrors how low-pH conditions in solution stabilize the same mesomeric form, establishing a direct conceptual link between wet-chemical and solid-state synthesis. We then extend this approach to other nitridocarbonate compounds to show that chemical descriptors such as ionic radius and hardness can predict which materials likely undergo similar pressure-induced transformations. This work highlights how mechanochemistry provides a new control lever for tuning mesomeric and electronic behavior in solids, expanding synthetic possibilities and establishing a broader, force-based design framework in solid-state chemistry.



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