



# CMCC Mechanochemistry Discussions

## Online Seminar Series

### *Probing Mechanochemical Reactions at Sliding Interfaces by Ab Initio and Machine Learning Simulations for the Design of Lubricants*

Livestreaming at  
10:00 AM (CT)  
THURS., July 17, 2025

on the CMCC YouTube Channel:

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



Prof. M. Clelia Righi  
University of Bologna, Italy  
<https://tribchem.it/>

Tribochemical reactions, involving lubricant or environmental molecules, are activated at the interface between two solids in relative motion. Key factors that distinguish them from mechanochemical reactions are the persistent, load-induced molecular confinement at the buried interface and the shear-induced atomic intermixing. These processes are crucial for the functionality of both solid and liquid lubricants under boundary lubrication conditions, where additives molecules directly react with solid surfaces.

To design environmentally friendly additives, it is important to understand the activation mechanisms and pathways of tribochemical reactions. However, real-time monitoring of the sliding interface is challenging experimentally. Simulations can play a key role here, in particular those based on a quantum-mechanical approach, which allows for an accurate description of the material behavior in conditions of enhanced reactivity.

I will describe how we used ab initio and machine learning-informed molecular dynamics (ML-MD) to identify key tribochemical mechanisms for the performance of both commercial and next-generation lubricants. In particular, I will show that the tribologically-induced dissociation of water molecules can promote the passivation of reactive carbon dangling bonds formed during rubbing and prevent the degradation of the lubricating properties of widely used solid lubricants such as diamond-like carbon (DLC) and graphite.

I will also show that slippery 2D materials can form in situ via tribochemical reactions. For example, a new route to generate transition metal dichalcogenides involves sprinkling chalcogen nanopowders onto sliding surfaces coated by metal films and graphene can be obtained through mechanochemically-induced polymerization of aromatic molecules of plant origin, leading to superlubricity. Finally, I will show that large-scale ML-MD can be used to perform in silico experiments to identify "green" additives able of improving the performance of water-based lubricants as a cleaner, sustainable alternative to petroleum oils.



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