FACOLTÀ DI SCIENZE MATEMATICHE, FISICHE E NATURALI
DIPARTIMENTO DI MATEMATICA E FISICA "NICCOLÒ TARTAGLIA"

Computational (Nano)Tribology and Materials to Reduce Friction

Introduce:
Luigi SANGALETTI, Università Cattolica del Sacro Cuore

Interviene:
Maria Clelia RIGHI
Department of Physics, Informatics and Mathematics, University of Modena and Reggio Emilia

Abstract
One of the main difficulties in understanding friction is related to the complexity and variety of phenomena that take place at the buried interface, which is not easily accessible by experiments. Simulations can, thus, play a crucial role in this context. In particular those based on quantum mechanics, which is essential to accurately describe the materials behavior in conditions of enhanced reactivity as those imposed by the mechanical stresses applied. I will present three examples where this approach has been successfully applied:

i) We monitor in real time the tribochemical reaction of graphene with water molecules. Our simulations unravel the important role of graphene edges and provide a relevant insight to understand the effects of humidity on the lubricity of graphitic systems, which I will discuss in comparison with MoS2, another important solid lubricant affected by humidity in opposite way.[1,2]

ii) Graphene and other carbon-based nanostructures are known to provide remarkable friction and wear performances, but need a continuous replenishment at the sliding interface. By means of ab initio molecular dynamics simulations we demonstrate a process of tribo-catalysis, where graphene is obtained from methane molecules confined at sliding Ni interfaces.[3]

iii) We perform a high-throughput screening of solid interfaces and find a correlation between the frictional forces and the electronic charge redistribution occurring during the relative displacement of two surfaces in contact. This suggests unconventional ways of measuring friction and explains a key mechanism of lubricant materials.[4]

[1] P. Restuccia, M. Ferrario and M. C. Righi, *Real-time monitoring of graphene edges passivation by water: Insights into the lubricity of graphitic materials*, submitted (2018).
[2] G. Levita and M. C. Righi, *Effects of water intercalation and tribochemistry on MoS2 lubricity: an ab initio molecular dynamics investigation* ChemPhysChem, **18**, 1475 (2017).
[3] Giovanni Ramirez, Osman Eryilmaz, Jianguo Wen, G. Fatti, M. C. Righi, and Ali Erdemir *In-Operando Conversion of Methane into Graphene and Other Carbon Nanostructures on Catalytically Active Sliding Surfaces*, submitted (2018).
[4] M. Wolloch, G. Levita, P. Restuccia, M. C. Righi, *Interfacial charge densities and their connection to adhesion and frictional forces*, Phys. Rev. Lett. **121**, 026804 (2018).

Seminario

Giovedì 6 giugno 2019
Sala Riunioni, ore 11.00-13.00
Via dei Musei 41 - Brescia

UNIVERSITÀ CATTOLICA del Sacro Cuore