Department of Physics

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Colloquia

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Computational (nano)tribology and materials to reduce friction

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.

We apply state-of-the-art methods used in computational physics/chemistry to unravel fundamental mechanisms of friction and design lubricant materials. I will present three examples:

i) We show that the adhesion and frictional forces are dictated by the electronic charge redistribution occurring due to the relative displacements of the two surfaces in contact. This suggests unconventional ways of measuring friction and explains a key mechanism to reduce adhesive friction exploited in lubricant additives.

ii) We apply, for the first time to our knowledge, Quantum Mechanics/Molecular Mechanics (QM/MM) simulations to tribology. 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 in graphitic systems, which I will discuss in comparison with MoS2, another important solid lubricant affected by humidity in opposite way.[2,3]

iii) Graphene and other carbon-based nanostructures are known to provide remarkable friction and wear performance, but need a continuous replenishment atbthe sliding interface. By means of ab initio molecular dynamics simulations we demostrate that the dissociative extraction of graphene is possible from methane molecules confined at sliding Ni interfaces.[4]

May 15
Wednesday

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References:
[1] M. Wolloch et. al., Phys. Rev. Lett. 121, 026804 (2018).
[2] G. Levita et. al., ChemPhysChem, 18, 1475 (2017).
[3] P. Restuccia et. al., submitted (2018).
[4] Giovanni Ramirez et. al., submitted (2018).

M. Cleila Righi is an Associate Professor at the Physics Department of the University of Modena and Reggio Emilia, where she coordinates a working group on computational tribology. She has a deep background in computational material design, surface/interface physics and nanoscience. She has experience in several methods to study materials properties at multiscales, including Density Functional Theory, ab initio and classical molecular dynamics and kinetic Monte Carlo.
She started her research activity on computational materials at the International School for Advanced Studies (SISSA) in Trieste. During her Ph.D. she studied materials growth with a multiscale approach. As postdoctoral fellow at the Physics Department of Unimore and at the CNR Institute of Nanoscience she acquired experience in the study of 2D materials, molecules-surface interactions and molecular dynamics methods.
In 2008 she started an independent research activity in nanotribology and tribochemistry. She collaborates with international research institutes and industries. She is part of the editorial board of Scientific Reports, Lubricants, and Lubrication Science.

The Department of Physics Seminars are designed to address a non-specialist, broad audience and introduce topics of contemporary research through lectures by leading experts. We warmly invite all members of the student body, including undergraduates enrolled in any programme.

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