

## Lubrificanti e materiali per ridurre l'attrito: Potenzialita' del computational material design

**M. Clelia Righi**

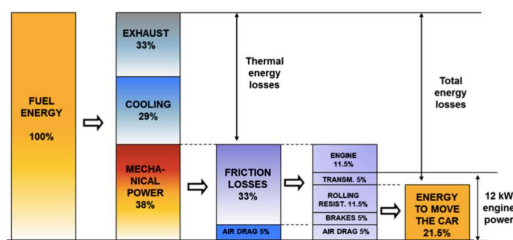
[www.tribchem.it](http://www.tribchem.it)

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### impact of friction on energy and environment



**one fifth of all the energy produced worldwide is used to overcome friction**

**There are 612 million cars in the world today**

K. Holmberg and A. Erdemir, FME Transactions 43, 181 (2015)

**Just a 10% friction reduction in every car engine will produce**

- > **fuel savings**  
385 billions liters/year
- > **CO<sub>2</sub> reduction**  
0.7 billions tonnes/year



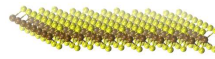
## Materials: technologies nowadays available to reduce friction



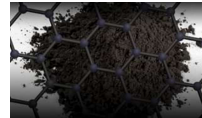
### Lubricants

- **Liquid lubricants:** base oil + lubricant additives

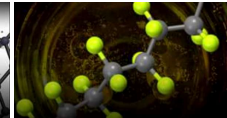
- **Solid lubricants**



MoS<sub>2</sub>

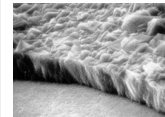
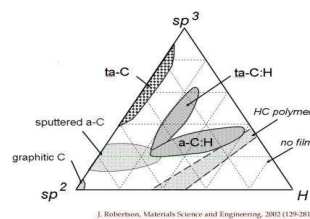


graphite



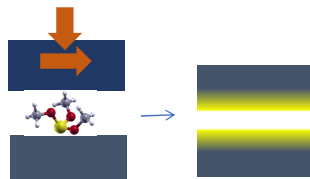
PTFE

**Coatings**  
Hard or superhard materials that reduce friction and wear



diamond like carbon

## computational tribochemistry



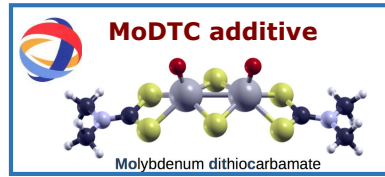
**stress-assisted chemical reactions**  
rule the functionality of lubricants



**monitoring tribochemical reactions**  
difficult by experiments

- **simulations play a crucial role** to real-time monitoring the sliding buried interface
- a **quantum mechanical approach is essential** for an accurate description of the chemical processes under extreme conditions
- *ab initio* molecular dynamics used **for the first time** in tribology

**industrial projects**



Sophie Lohele'



Seiji Kajita

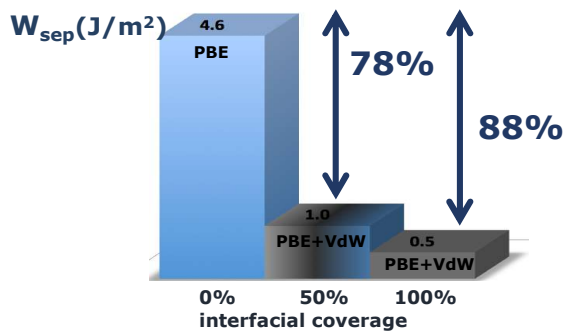
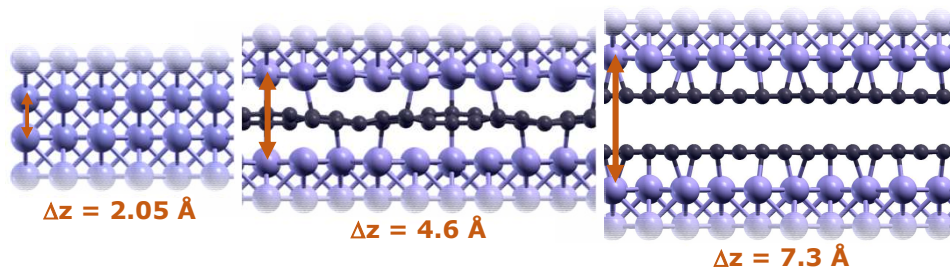
**diamond/DLC with TOYOTA Central R&D Labs**

**Ab initio Green Functions MD**

$$v_{surface}(t) = \int g(t-t') F_{ext}(t') dt' + v_{thermal}$$

① Green's function (GF) ②

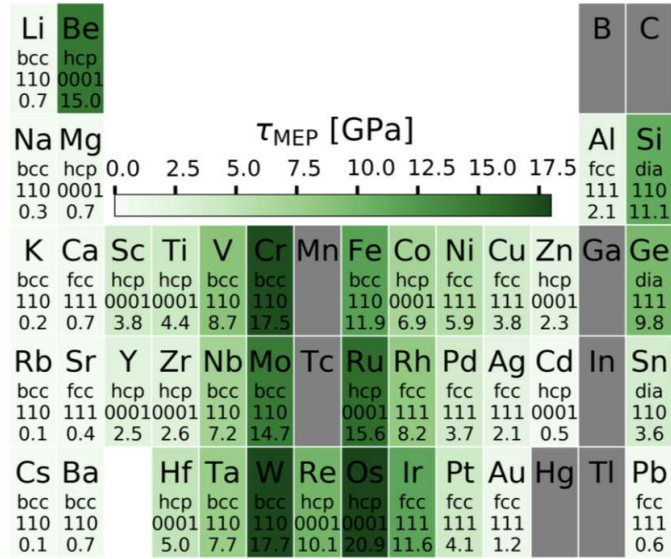
**graphene at iron interface**



Iron surfaces coated by graphene become almost inert and present very low adhesion

P. Restuccia, M. C. Righi, Carbon 106, 118 (2016)

## resistance to sliding



## contacts

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