Guilherme Vilhena, Ruben Perez
Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain
guilhermevilhena@gmail.com

Atomistic understanding of the mechanical properties of bio-molecules

In the past decades, single molecule (SM) experiments have allow us to unravel many different complex mechanisms at a molecular level. Interestingly, its achievements may be found in very disparate research fields, e.g.: unraveling the origins of superlubric (lack of) friction between some solid surfaces, controlling chemical reactions with atomic resolution, understanding the operation of molecular motors present in living cells, and most recently they have also shown the ability to track relevant metabolic information of living cells (volume, size, mass) with an unprecedented time and spacial resolution. The ubiquity of these findings reminds us of the general interest in controlling processes at a molecular scale while extracting relevant observables when doing so.

Despite their undisputed merit, associating mechanical response of a given molecule with conformational changes at an atomic level it is still an utmost challenging task. In this talk, we will give a birds eye view of how atomically detailed molecular dynamics (MD) simulations allow us to not only qualitatively reproduce the results obtained in these experiments but also it allow us to overcome this SM limitation particularly by providing insights on how deformations/motions occurring at the atomic scale relate to their physical properties. In particular, we shall show how these simulations allow us to understand: how a single atom may drastically alter mechanical properties of a molecule (DNA/RNA)[1]; how internal molecular degrees of freedom allows us to tune friction and adhesion at a molecular level in vacuum conditions [2,3,4]; how the complex force/indentation curve obtained in Atomic-Force-Microscopy experiments of complex biomolecules conducted in liquids may be deconvoluted into simpler atomistic mechanisms, namely local molecular elasticity and (hydrophobic) adhesive effects[].

References

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Figures

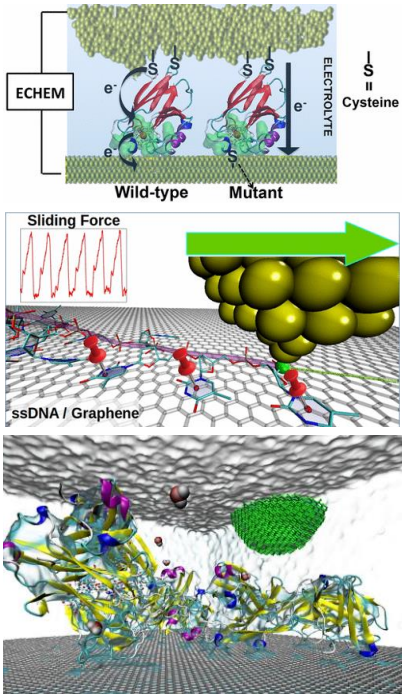

Figure 1: Atomistic representation of: (top) how single point mutation in a protein drastically affect its electronic properties [5]; (middle) sliding a single-stranded DNA molecule over a graphene surface in vacuum while measuring the corresponding friction force [4]; (bottom) virtual atomic force microscope – atomistic simulation of the indentation of an antibody (IgG) deposited over a graphene surface with the system fully embedded in water.