UNIVERSITÀ DEGLI STUDI DI PADOVA

DiSC

Lunedì **11 novembre 2019** alle ore **12:00** presso l'aula L2

il Dott. Patrick Charchar

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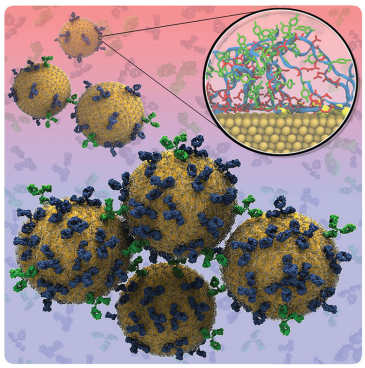
terrà il seminario dal titolo:

Exploring the gold–nano–bio interface through molecular simulations

Biologically compatible noble metal nanoparticles are envisaged to become an integral component in clinical and diagnostic biomedicines due to their novel and advantageous physiochemical properties. Advances over the past few decades have made it possible to synthesize nanoparticles with atomic precision and specific functionalizations, allowing experimentalists multiple levels of control to create exciting materials that have tailored physical and optical properties as well as selective and specific chemical attributes.

To effectively engineer gold nanomaterials ultimately destined for applications within complex *in vitro* and/or *in vivo* environments, it is critically important to understand and regulate the fundamental interactions occurring at the gold–bio interface. To provide this information, computational approaches are instrumental as they can complement, elucidate and predict empirical data with spatial and temporal resolutions not yet achievable in the laboratory.[1]

The talk will discuss our recent progress using classical molecular dynamics, synergistically with experimental data from our collaborators at Imperial College London, to gain atomistic structure–property relationships of peptide-coated gold nanoclusters[2] (< 2 nm) and nanoparticles[3] (c.a. 20–60 nm). The outcomes of these works improve our understanding of the gold–bio interface and contribute to the design of the next generation of biomaterials with broad applications in the fields of bioimaging and biosensing.



Computational modelling is a virtual microscope used to probe complex nano–bio interfaces. Reproduced with permission.[1] Copyright 2016, Wiley-VCH Verlag GmbH & Co.

1. Charchar, P.; Christofferson, A. J.; Todorova, N.; Yarovsky, I. *Small* **2016**, *12*, 2395.
2. Lin, Y.*; Charchar, P.*; Christofferson, A. J.; Thomas, M. R.; Todorova, N.; Mazo, M. M.; Chen, Q.; Doutch, J.; Richardson, R.; Yarovsky, I.; Stevens, M. M. *J. Am. Chem. Soc.* **2018**, *140*, 18217. (*Equally contributing authors)
3. Andresen, H.; Mager, M.; Grießner, M.; Charchar, P.; Todorova, N.; Bell, N.; Theocharidis, G.; Bertazzo, S.; Yarovsky, I.; Stevens, M. M. *Chem. Mater.* **2014**, *26*, 4696.

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Stefano Corni

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