

<b>Title</b>	<b>Multiscale simulations of protein-surface and protein-nanoparticle interactions</b>
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### Project description:

Protein-surface & protein-nanoparticle interactions are central to several material science and bio-oriented systems, such as enzymatic biofuel cells (electric power by organics fuels), guiding self-assembling at the nanoscale with material-specific proteins, nanoparticle effects on protein aggregation. The PhD project consists in extending the computational tools developed by our group, and/or to apply them to problems of biotechnological/material science relevance. A MSc background in Computational Chemistry or Physics is helpful but not mandatory.

### Publications:

1. L. Bellucci, G. Bussi, R. Di Felice, S. Corni *Fibrillation-prone conformations of the amyloid- $\beta$ -42 peptide at the gold/water interface* *Nanoscale* 9, 2279 (2017)
2. Ozboyaci, M., Kokh, D.B., Corni, S., Wade, R.C. *Modeling and simulation of protein-surface interactions: Achievements and challenges* *Quart. Rev. Biophys.* 49, e4 (2016)
3. L.B. Wright, J. P. Palafox-Hernandez, P.M. Rodger, S. Corni, T.R. Walsh, *Facet selectivity in gold binding peptides: exploiting interfacial water structure* *Chem. Sci.* 6, 5204 (2015)
4. G. Brancolini, A. Corazza, M. Vuano, F. Fogolari, M. C. Mimmi, V. Bellotti, M. Stoppini, S. Corni, G. Esposito, *Probing the Influence of Citrate-Capped Gold Nanoparticles on an Amyloidogenic Protein* *ACS Nano* 9, 2600 (2015)

### Collaborations/Network:

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R.C. Wade, Univ. Heidelberg & HITS, DE  
G. Brancolini, CNR-NANO Modena, IT  
G. Esposito, Univ. Udine, IT & NYU, Abu Dhabi, UAE  
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