Modeling complex nanosystems for drug delivery, targeted therapy and imaging

Cristiana DI VALENTIN - *University of Milano Bicocca - NanoQlab*

In this talk, I will present an overview on our multiscale computational activity devoted to nanohybrid systems based on transition metal oxide nanoparticles (i.e. TiO_2 and Fe_3O_4) and graphene-based materials for biomedical applications. Atomic models of realistic size (2-4 nm, i.e. 800-4000 atoms) are used to simulate, at a quantum mechanical level of theory in combination with molecular mechanics and classical molecular dynamics, the structural, electronic and magnetic properties of these nanosystems, their interaction with light and with the aqueous environment, considering physiological conditions. Surface functionalization with stabilizing polymers or functionalizing molecular species for drug delivery, targeted photodynamic therapy and imaging is then tackled. The description of complex protein corona effects and ligand/receptor interactions demands a more efficient exploration of the configuration space with techniques like umbrella sampling and metadynamics and the complementary analysis by means of machine learning techniques.