Materials Science & Engineering Seminar Series

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Designing ligand-functionalized nanoparticles: Insights from theory and simulations

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Abstract:
Designing new functional materials as well as optimising the performance of existing ones necessarily requires a solid understanding of the physical principles governing their behaviour. Without this knowledge, their development would necessarily follow an empirical "trial and error" route, with very little success chances (and high costs), especially for complex materials where the number of parameters determining their behaviour is large. In this regard, theory and computational simulations can serve as an important tool to guide experiments, as well as to screen *a priori* the effect of specific parameters choices in a controlled environment. Following this line, I will present in this talk our recent results in the theoretical description of ligand-functionalized nanoparticles (with emphasis on DNA-coated colloids) [1,2,3,4]. These materials are studied for various applications, including the self-assembly of photonic structures, DNA-biosensors and vectors for drug-delivery, and I will show how our models can and have been used not only to understand their behaviour and guide their optimisation, but also to suggest completely new designs resulting in new, unprecedented properties [1,4].

Bio:
After my undergraduate (2005) and Master studies (2007) in Materials Science at the University of Milano-Bicocca (Italy), I moved to the UK at Imperial College London, where I obtained my PhD in Materials Science (2010) studying atomistic approaches to describe solid-liquid interfaces in alloys under the supervision of Prof. Mike Finnis and Prof. Peter Lee. I then moved from "hard" to "soft" matter during my first postdoc, at the Chemistry Department of the University of Cambridge, where I began to study DNA-coated colloids and their theoretical description in the group of Prof. Daan Frenkel. In 2013, thanks to an Alexander von Humboldt Research Fellowship, I moved to Germany at the Humboldt University of Berlin, where I kept working on the properties of various types of functionalized nanoparticles, nanogels and their applications. Very recently, I joined the Institute for Soft Matter Research, part of the Beijing University of Chemical Technology (China), as a PI and group leader of the Computational Soft Matter Group.

Doherty Hall 2210, 11:30AM
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