PhD second year report

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1 Research Activity

My research activity is within the Nanobiocomp research group, where we investigate the behaviour of matter at the nanoscale by computational tools. In my work I mostly apply molecular dynamics (MD) simulations to the study of nanoparticles and nanoalloys, with regard to the different structures and processes of growth and diffusion.
One important field of research is that of multi-component aggregates and their highly tunable properties, with many different possible applications. We established a general theoretical framework for the prediction of stable icosahedral structures as a way to deal with the great configurational complexity of these systems. This we did by assembling concentric shells of different chiral and achiral types, consisting of particles of different sizes. We mapped shell sequences into paths in the hexagonal lattice, working with a method first introduced by Caspar and Klug for the study of viruses. We found simple and general rules for designing a wide variety of magic icosahedral structures, which could naturally be obtained by a process of growth, based on the optimal size-mismatch between particles in the different shells. The predictions of our design strategy are confirmed by MD simulations of growth in a variety of binary systems such as Ni@Ag, Co@Ag, Cu@Ag, Ni@Au, Co@Au and Fe@Au. Density functional theory calculations were also performed in a variety of binary and ternary systems, selected on the basis of a good size-mismatch and reasonable cohesive energy.
We did a work on the diffusion of an atom on the surface of a metal nanoparticle, which we started with the purpose to explain the very smooth process of growth of chiral icosahedra. What we observed is that while on a smooth surface an atom (of the same atomic species of the surface) typically 'jumps' from one facet to the next, 'exchange' prevails as a mechanism for mass transport near a sharp edge. This means the atom take its place on the edge sending on the next facet the atom that was previously there. This way we

can explain why both the chiral icosahedron and the tetrahedron allows for a very regular process of growth: newly added atoms easily diffuse on both surfaces, in one case by 'jump' and in the other by 'exchange'.
Finally, we began an investigation on the pressure at the center of octahedral and icosahedral nanoparticles, made either of silver or of copper, with the aim to verify and generalize the Laplace rule.

2 Exams

Exam given: Fisica statistica dei sistemi fuori equilibrio (by Nicodemo Magnoli): 6 cfu.
Exam given: Atomic force spectroscopy (by Annalisa Relini): 3 cfu.

3 Publications and contributions

Article "Path-based packing of icosahedral shells into multi-component aggregates" by Nicolò Canestrari, Diana Nelli, Riccardo Ferrando, submitted, preprint on arXiv: https://doi.org/10.48550/arXiv.2406.07137.
Talk "Icosahedra" given at: IIT Genova, 1/12/2024.
Talk "Icosahedra" given at: Rome, kick-off meeting of the project PINENUT, within PRIN2022.
Talk "Diffusion on metal nanoparticles" given at the International Meeting on Nanoalloys 2024 in Genova.