"Development of a Predictive Framework for Programmable Nanoscience"

There is an opening for 2 PhD positions at the group of Alex Travesset at Iowa State University for developing mean field and simulation models for the prediction of nanoparticle assembly. This project will be developed in close collaboration with the group of Mario Tagliazucchi at Universidad de Buenos Aires and will include collaborations with different experimental groups in the USA and Switzerland.

Nanoparticles are solids consisting of a small number of atoms, in such a way that at least one of the three dimensions is of the order of a few nanometers ($1nm=10^{-9}$ m). Quantum dots, for example, are a type of nanoparticle that emits light in different colors depending on their size. Over the last decade a new paradigm for material design has emerged, where instead of directly assembling atoms or molecules into materials, first nanoparticles are made, and then, the nanoparticles themselves are assembled into functional materials. This allows an unprecedented level of control, but also, the ability to design materials with new functions, with potential for game changing applications in energy harvesting technologies, quantum information, new display devices, as well as medical imaging, just to name a few.

This project aims at providing a robust platform for designing nanoparticle based materials. Driven by the ability to synthesize large numbers of nanoparticles with diverse sizes, composition and the implementation of a broad range of strategies to assemble them in actual materials, the field has had an extraordinary experimental progress over the last decade. What is needed to accelerate this process of discovery is a comprehensive computational/theoretical framework that will identify what combination of design parameters will lead to materials with new functions. The project aims to fill this gap by developing a general framework (mean-field model), complemented with numerical simulations and other theoretical advances that will enable the prediction of structure and in this way, a rational exploration of the optimal parameters for designing new materials. The developed framework will be made available through a software package for the benefit of the entire community. Examples of some preliminary results are provided in the references below.

This is a very exciting project that we expect will have a large long-term impact. The optimal candidate should have interest in both theory as well as computation, including software development. Interested candidates can contact

Prof. Alex Travesset, Iowa State University, USA, **trvsst@ameslab.gov**

Prof. Mario Tagliazucchi, Universidad de Buenos Aires, **mario.tagliazucchi@gmail.com**

SELECTED REFERENCES

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