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Research domain(s), discipline(s)/sub-discipline(s)

Soft Condensed Matter; Self and Directed Assembly

Title of Response

First Principles Predictions of Nanoparticle Asssemblies

Abstract

The last decade has witnesses a spectacular progress in our ability to create and assembly nanoparticles into relevant materials. Current and future computational capabilities, coupled with conceptual advances will enable the goal of predicting the conditions under a certain nanoparticle assembles into some desired structure.

Question 1 (maximum 400 words) – Data-Intensive Research Question(s) and Challenge(s). Describe current or emerging data-intensive/data-driven S&E research challenge(s), providing context in terms of recent research activities and standing questions in the field. NSF is particularly interested in cross-disciplinary challenges that will drive requirements for cross-disciplinary and disciplinary-agnostic data-related CI.

Current data intensive problems are the classification of all possible superlattice structures consisting of two or more nanoparticle species and their realization in practical materials. Even with simple models, such as particles interacting with Lennard-Jones potentials, a binary system shows a bewildering number of equilibrium crystalline phases. When the considerations expand to including metastable phases, there are tens of thousands of phases present. And this is only a very simple case, as systems including more than two species are necessary to consider to bring the full potential of nanoparticle materials into fruition. These type of efforts are cross-disciplinary as they involve physics, chemistry, materials science and mathematics, with a strong computer science background.

Question 2 (maximum 600 words) – Data-Oriented CI Needed to Address the Research Question(s) and Challenge(s). Considering the end-to-end scientific data-to-discovery (workflow) challenges, describe any limitations or absence of existing data-related CI capabilities and services, and/or specific technical and capacity advancements needed in data-related and other CI (e.g., advanced computing, data services, software infrastructure, applications, networking, cybersecurity) that must be addressed to accomplish the research question(s) and challenge(s) identified in Question 1. If possible, please also consider the required end-to-end structural, functional and performance characteristics for such CI services and capabilities. For instance, how can they respond to high levels of data heterogeneity, data integration and interoperability? To what degree can/should they be cross-disciplinary and domain-agnostic? What is required to promote ease of data discovery, publishing and access and delivery?

The are several requirements for these research questions and challenges. First of all, other than isolated efforts by different groups, the field does not still exist. This implies an absence of common tools and standards. A first step would consist of building a repository of all existing data structures describing all nanoparticle assemblies, both experimentally and computational, according to certain standards, to where existing applications, in regards to classification and identification of space groups, quasicrystals, etc.. would be applied. There is also a need to use and develop software: this includes machine learning and other tools aimed at the classification with relevant parameters of all possible structures for given nanoparticle specifications such as number of species and their shapes. Also, optimization of their structural and electronic, optical, catalytic or transport properties. This will require software of high quality and accessibility for all researchers around the globe.

Question 3 (maximum 300 words) – Other considerations. Please discuss any other relevant aspects, such as organization, processes, learning and workforce development, access and sustainability, that need to be addressed; or any other issues more generally that NSF should consider.

The main challenge in regards to workforce is the development of a new class of scientists that being proficient in the science, they are also on top of professional computer science tools. Software sustainability is also another challenge, as often, there are funding sources available for software, but not for its sustainability.

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