Contribution ID : **198** Type : **Poster Presentation**

Multiscale Computational Design of Luminescent Nanoparticle Supercrystals

The project will introduce a rational design of ligands to finely tune nanoparticle shell thickness and density, complemented by functionalization strategies for supercrystals aimed at reinforcing interparticle interactions and reducing inter-nanoparticle spacing. Ab initio simulations based on density functional theory (DFT) are employed to predict electronic, structural, and magnetic properties of novel materials. First-principles simulations also support the design of heterostructures with tailored quantum behaviors, guiding experimental synthesis and characterization.. Overall, this theoretical framework supports the rational design of next-generation superconducting nanomaterials. We integrates advanced computational techniques with a multiscale modeling to investigate superconductivity at the nanoscale, by playing with nanoparticles size and surface chemistry toward a library of highly stable and strongly coupled structures. To this end, we aims to overcome the vulnerabilities of these materials through the assembly of nanoparticles into supercrystals, development of 3D supercrystals, optimization of ligand design. The formation of supercrystals will improve experimental testing in optoelectronic devices.

1. Kovalenko, M. V., et al., ACS Nano 2015, 9, 1012-1057.
2. Vovk, I. A., et al., Physical Chemistry Chemical Physics 2018, 20, 25023-25030.
3. Krieg, F., et al., ACS Energy Lett. 2018, 3, 641-646.
4. Tong, Y., et al., Adv. Mater. 2018, 30, 1801117.

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