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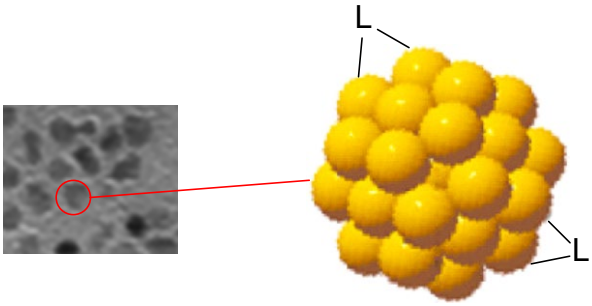
Theoretical study of the influence of Ligand-Metal interaction in nanoparticles growth

Since the advent of nanoscience, the grail of chemists is to perfectly and reproducibly elaborate nanoparticles (NPs) of fully defined size, shape, polydispersity, and surface state. It implies a total control of the experimental parameters affecting the synthesis. NPs may be prepared using a physical or chemical route. Among the latter, the synthesis of colloidal metallic nanoparticles can involve a precursor complex, which is reduced in the presence of stabilizing ligands. Such ligands prevent the nanoparticles' coalescence in solution by the formation of a shell of organic dispersant around them.

Using Wide Angle X-Ray Scattering to characterize the metal-metal distances, the group of Dr. M. Kahn (Toulouse) have evidenced two families: in the nanoparticle core, the metal-metal distance is that of the bulk, while a longer distance is observed for some atoms at the surface. We hypothesize that these larger distances are due to metal atoms bridged by the ligand (Scheme 1). Interestingly, this larger distance is directly correlated with the Metal/Ligand ratio used in the synthesis.



Nanoparticle

Scheme 1

The goal of this internship is to analyze the Metal-Ligand bond using quantum chemical tools (such as Atoms In Molecules, Electron Localization Function…).[1] This will help us to understand the link between the ligand coordination and the metal-metal bond distance and the correlation between the metal/ligand ratio and the metal-metal distance evolution.

Required Skills: The successful candidate should have a background in physical chemistry with basic knowledge in organometallic chemistry and spectroscopy. No programming knowledge is needed.

Bibliography

[1] Wang, Y.; Coppel, Y.; Lepetit, C.; Marty, J.-D.; Mingotaud, C.; Kahn, M. L. Anisotropic Growth of ZnO Nanoparticles Driven by the Structure of Amine Surfactants: The Role of Surface Dynamics in Nanocrystal Growth. *Nanoscale Adv.* **2021**, *3* (21), 6088–6099. https://doi.org/10.1039/D1NA00566A.
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