

# RCMS & GTR Seminar

## Electron and spin (de)localization in polynuclear complexes based on a triphenylene tris dioxolene bridge, experiment and theory



Prof. Talal Mallah

(*Université Paris-Saclay*)

Date: 24th June (Mon.) 10 : 30~

Venue: 野依記念物質科学研究館ケミストリーギャラリー

A trinuclear ( $\text{Ni}_3$ ) complex is assembled from the reaction of Ni(II) capped with a blocking tris-pyrazolyl borate tridentate ligand and deprotonated tris-catecholate hexahydroxytriphenylene ( $\text{H}_6\text{HHTP}$ ).<sup>1,2</sup> The crystal structure and the magnetic data are consistent with a three-electron oxidized bridge leading to the tris-semiquinone ([sq-sq-sq]) form with a single unpaired electron. The single unpaired electron is found to be mainly localized on one of the OCCO moieties of the tris-semiquinone. Upon one and two-electron reduction, the molecule switches to the [sq-sq-cat] (cat stands for catecholate) state and then to the [sq-cat-cat] one detected by EPR. Using a bidentate capping ligand allows the assembly of a hexanuclear ( $\text{Ni}_6$ ) complex. The bridging ligands are in the semiquinone state. The electrochemical properties show two one-electron oxidation and reduction processes that can be rationalized as due to the interaction between the non-innocent bridging ligands as supported by wave function based theoretical calculations.



Contact Kunio AWAGA  
awaga.kunio.h8@f.mail.nagoya-u.ac.jp