UDESC
UNIVERSIDADE
DO ESTADO DE
SANTA CATARINA

JOINVILLE
CENTRO DE CIÊNCIAS
TECNOLÓGICAS

PROGRAMA DE PÓS-GRADUAÇÃO EM QUÍMICA
SEMINÁRIOS

2021/2 – PPGQ / SEM I e II

DATA:
06/10/21

PALESTRANTE:
Prof. Dr. Claudio Verani*

INSTITUIÇÃO:
WSU - Wayne State University, Estados Unidos (Departamento de Química)

TÍTULO DA PALESTRA:
Electron transport in electrode|metallosurfactant junctions.

RESUMO:

The Verani Group is invested in the development of new concepts in molecular electronics, a field that aims to develop molecular-size electronic components such as transistors, diodes, and resistors. We are developing amphiphilic coordination complexes [M(L)] known as metallosurfactants. When these species are deposited in between two gold electrodes, they form assemblies described as $Au_1|(ML)|Au_2$ junctions that can promote *directional electron transport*:

$Au_1 + e^- |(ML)o| Au_2$ à $Au_1 + |(ML) + e^- | Au_2$ à $Au_1 + |(ML)o| Au_2 + e^-$

This directional transport of electrons is called *current rectification*, and the metallosurfactants behave as *molecular diodes*. To date we have synthesized, characterized, and analyzed several metallosurfactants containing $3d^1$ VO^{IV}, $3d^3$ Cr^{III}, $3d^4$ Mn^{III}, $^{HS}3d^5$ Fe^{III}, $3d^9$ Cu^{II}. In this talk, we will introduce the methodology, discuss the experimental work, and explain the intricate mechanistic insights obtained for each of these electronic configurations.

In the process, we will utilize fundamental concepts of coordination chemistry such as electronic configurations, coordination numbers, redox behavior of metals, ligand fields, and molecular orbital theory. We propose that rectification in metallosurfactants depends on (i) molecular asymmetries enforced by five-coordinate ligand fields associated with orbital distortions; (ii) structural asymmetries enabling localized placement of the LB film closer to one of the electrodes, and (iii) the matching of the energies between electrode Fermi levels and the SOMOs of the metallosurfactant.

Funding: US National Science Foundation.

* **Claudio Verani** got his M.Sc. (1997, honors) at the Universidade Federal de Santa Catarina in Brazil, where he synthesized bioinorganic models for copper enzymes. His Ph.D. came from the Max-Planck Institute for Bioinorganic Chemistry and Ruhr Universität-Bochum in Germany, where he developed experimental models to understand magnetic coupling in heterometallic species. He moved to the US in 2000 for postdoctoral work at the Johns Hopkins University, modelling aspects of dioxygen activation by Cytochrome-c-oxidase. At Wayne State since 2002, he was promoted to associate professor in 2008 and to professor in 2013. He is also serving as associate dean for research at the WSU - College of Liberal Arts and Sciences since 2017. He and his group utilize a multidisciplinary approach to develop (i) new concepts in molecular

electronics and (ii) Earth-abundant catalysts for water splitting. In his free time, he enjoys the company of wife, daughter, and dog, tries to play music, and reads about archaeology, history, and politics.