Short bio:

Renaldo T. Moura Jr. (1983 -), received his Ph.D. from Federal University at Pernambuco (Universidade Federal de Pernambuco – UFPE, Brazil) in 2013 and was a pos-doc during 2013-2016 at the Department of Fundamental Chemistry (Departamento de Química Fundamental – dQF – UFPE, Brazil). Since 2016 he is an Assistant Professor at the Department of Chemistry and Physics (Departamento de Química e Física), Federal University at Paraíba (Universidade Federal da Paraíba), Areia, PB, Brazil. He is a Visiting Professor at the Computational and Theoretical Chemistry Group (CATCO) at Southern Methodist University (SMU) in Dallas, Texas, USA during 2022-2023. He served as chair of the Department of Chemistry and Physics from 2019 to 2022. Prof. Renaldo's scientific interests cover the development of theoretical and computational methods for inorganic and physical chemistry, particularly for numerical methods, chemical bonding, and molecular spectroscopy. He has supervised and co-supervised 3 Ph.D., 7 MSc, and 11 undergraduate students in the Chemistry Graduate Programs. Currently, he is co-supervising 02 Ph.D. and supervising 04 MSc students. He is the author of 03 book chapters and about 27 papers in journals with impact factors.

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Abstract

Computational studies on lanthanide compounds' luminescent properties are important for designing new luminescent materials. However, the development of suited computational methods and protocols is still in its infancy. In this seminar, we will discuss a new computational protocol for analyzing the luminescent properties of Ln(III) based compounds. A brief explanation of underlying theories and models will be presented, namely: local vibrational mode (LVM) theory; expansions on the bond overlap model (BOM); and advances in intramolecular energy transfer (IET) rates determination will be shown up.