# "ACCURATE QUANTUM CHEMICAL METHODS FOR EXCITED ELECTRONIC STATES AND TRANSITION-METAL COMPOUNDS"


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## April 09, 2021 (Friday)
## 12pm (BRT time) - Google Meet

**ORGANIZATION:**

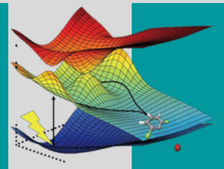
**Prof. Dr. Antonio Carlos Borin**

Instituto de Química, Universidade de São Paulo (USP), SP, Brazil

**INFORMATION AND REGISTRATION:**

**ancborin@iq.usp.br**

**Registration**: send a message to ancborin@iq.usp.br
with the words "Laura Gagliardi – Virtual" on the "subject"
**Deadline:** April 07, 2021 (Wednesday), 06pm (BRT time)



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## ABSTRACT

### Accurate Quantum Chemical Methods for Excited Electronic States and Transition-Metal Compounds


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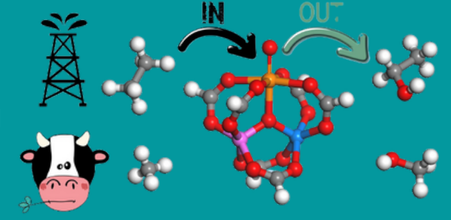
I will give an overview of the challenges that modern electronic structure theory faces in describing strongly correlated chemical systems from molecules to materials. Our latest progress in combining density matrix renormalization group with pair-density functional theory as a new way to calculate correlation energy [1] will be discussed, together with the recent development of density matrix embedding methods based on multireference solvers for molecules [2], [3] and materials [4]. Applications to compounds containing transition metals and excited states will be presented [5]. As an example, in the second part of my talk I will present our latest work on metal-organic frameworks (MOFs) [6].



[1] P. Sharma, V. Bernales, S. Knecht, D. G. Truhlar, and L. Gagliardi, Density matrix renormalization group pair-density functional theory (DMRG-PDFT): singlet–triplet gaps in polyacenes and polyacetylenes, Chem. Sci., 10, 2019, pp 1716-1723.

[2] M. R. Hermes and L. Gagliardi, Multiconfigurational Self-Consistent Field Theory with Density Matrix Embedding: The Localized Active Space Self-Consistent Field Method, J. Chem. Theory Comput., 15, 2019, pp 972-986.

[3] M. R. Hermes, R. Pandharkar, and L. Gagliardi, The Variational Localized Active Space Self-Consistent Field Method, J. Chem. Theory Comput., 16, 2020, 4923-4937.

[4] Hung Q. Pham, Matthew R. Hermes, L. Gagliardi, Periodic Electronic Structure Calculations with Density Matrix Embedding, Theory J. Chem. Theory Comput., 16, 2020, pp 130-140.

[5] P. Sharma, D. G. Truhlar, and L. Gagliardi, Magnetic Coupling in a Tris-hydroxo-Bridged Chromium Dimer Occurs through Ligand Mediated Superexchange in Conjunction with Through-Space Coupling, J. Am. Chem. Soc., 142, 2020, pp 16644-16650.

[6] J. G. Vitillo, A. Bhan, C. J. Cramer, C. C. Lu and L. Gagliardi, Quantum Chemical Characterization of Structural Single Fe(II) Sites in MIL-Type Metal Organic Frameworks for Oxidation of Methane to Methanol and Ethane to Ethanol, ACS Catal., 2019, 9, 2870–2879.