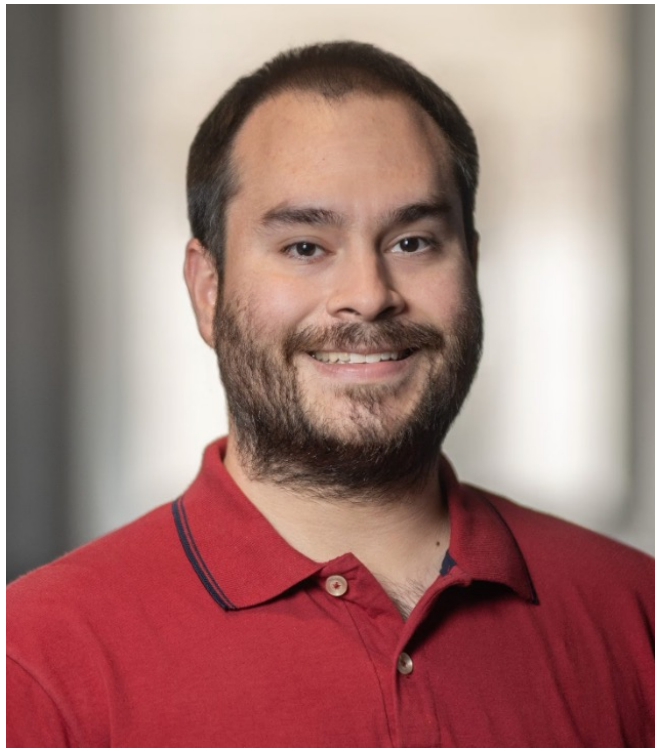
Leonardo dos Anjos Cunha, Ph.D.

Flatiron Research Fellow, Center for Computational Quantum Physics, Flatiron Institute

CCQ NYU
LIGHT-MATTER SEMINAR



Title: Photonic Observables as Probes for Dynamical Processes in the Polaritonic Regime

Abstract: Achieving control over molecular processes and properties is essential to chemical sciences as a whole. Light is usually an essential, albeit passive, ingredient to achieve control over chemical processes and reactivity. However, recent advances in optical confinement have granted a more active role to light in the task of controlling chemical properties. In the so-called strong-coupling regime, hybrid electron-photon states, or polaritons, emerge and are crucial to understanding changes in reactions yields[1], assisting in self-assembly[2], and modifying material properties.[3] These experiments have led to a flurry of new theoretical developments to model and better understand such new phenomena. Generalizations of traditional quantum chemistry methods, such as density functional theory[4] and coupled cluster theory[5], have been applied to study proton transfer reactions[6], and the behavior of van der Waals (vdW) interactions[7] in the strong-coupling regime. However, most of these studies focus only on analyzing energetic variations, such as reaction barriers, for systems strongly coupled to optical cavities. In this talk, we will give an overview of quantum chemistry methods for hybrid light-matter systems, such as QED-CI, QED-CC and QEDFT. We will then use these tools to analyze how photonic observables, such as the effective number of photons in a given state, can be used to capture dynamical effects, such as bond breaking and oscillations along the normal modes of a molecule.

References: **1.** *Angew. Chem. Int. Ed.,* 51.7 (2012): 1592-1596. , **2.** *J. Phys. Chem. Lett.,* 13.5 (2022): 1209-1214., **3.** *Science,* 354.6309 (2016): aag1992. 4. *Phys. Rev. A,* 90.1 (2014): 012508., **5.** *Phys. Rev. X,* 10.4 (2020): 041043., **6.** *J. Am. Chem. Soc.* 144.11 (2022): 4995-5002., **7.** *arXiv preprint arXiv:2209.07956* (2022).