



Speaker: Dr. Luca Argenti, University of Central Florida

From Atoms to Molecules: Theory on the Heels of
Attosecond Electron Dynamics

Friday, March 6, 1:30 pm, PSB 160/161

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Abstract: Attosecond science has made it possible to resolve photoionization processes and coherent electronic excitations in atoms and molecules in real time. *Ab initio* wave-function methods play a central role in this effort, as they are essential to describe multiple excitations and entanglement between photofragments. In this talk, I will illustrate the capabilities of the close-coupling method for simulating photoelectron and optical attosecond spectroscopies in atoms and molecules. In molecular systems, the main challenge is scalability with respect to both electronic correlation and molecular size. To address this problem, we have developed ASTRA, a new code based on transition density matrices, which we have applied to molecular transient absorption, charge migration, and sequential double ionization, in combination with surface-hopping methods.

BIO: Luca Argenti leads the Theoretical Attosecond Group at the Department of Physics, with secondary joint appointments at CREOL and the Chemistry Department. His group studies the time-resolved correlated electronic motion in polyelectronic atoms and molecules and develops numerical quantum-mechanical methods required for the reconstruction of this dynamics. LA earned his undergraduate degree in chemistry in 2001 from the University of Pisa (Italy, EU), concurrently with a Diploma from Scuola Normale Superiore of Pisa (SNS), and his Ph.D. in chemistry in 2008 from SNS. He was a Postdoctoral Fellow at Stockholm University (Sweden, EU) between 2009 and 2010, and at the Autonomous University of Madrid (Spain, EU) between 2010 and 2016. He began as an Assistant Professor at UCF in 2016, where he was promoted to Associate Professor in 2020.