



SoFlacs



Vol. 33, No. 1

South Florida Section American Chemical Society

January 2023



In-Person Section Meeting

Friday, January 20, 4:00 PM

330 Holmes Hall, Florida Gulf Coast University, Ft. Myers

Refreshments: 5-7 pm, 406 Holmes Hall

or Join by Zoom Meeting

<https://fgcu-edu.zoom.us/j/95680823205?pwd=NnFpRndicDhvb0Zzb0diQ2FTbWhjdz09>

Meeting ID: 956 8082 3205, Passcode: 679006

Dr. Daniel Lambrecht

Department of Chemistry and Physics, Florida Gulf Coast University

“May the force be with you” Understanding effects of non-covalent interactions on molecular structure, properties and reactivities

Abstract: Non-covalent interactions such as hydrogen bonding, van der Waals and electrostatic forces are sometimes thought of as secondary to covalent chemical bonds. However, interesting chemistry arises when non-covalent forces are strong enough to tip the balance towards altering the structure or reactivity of a molecule. This presentation discusses computational approaches for investigating the origins and magnitudes of non-covalent interactions to develop a bottom-up understanding of chemical structure and reactivity. A range of applications will be presented to showcase the utility of these insights, including the study and design of molecules with environmental applications such as the capture of pollutants and the study of solvent and ion effects on monomer reactivities relevant to polymer synthesis. For the first project, it is shown that the binding of pollutants can be systematically enhanced by tailoring the molecular structure based on insights from interaction energy studies. In the second spotlight, it is analyzed how counterion and solvent effects impact the reactivity and regioselectivity in bifunctional monomers as they undergo reactions with anionic nucleophiles.

Dr. Daniel Lambrecht studied chemistry in Düsseldorf, Germany and completed his graduate work in theoretical and computational chemistry with Prof. Christian Ochsenfeld in Tübingen, Germany. He continued with postdoctoral research with Prof. Martin Head-Gordon at the University of California. Dr. Lambrecht is an associate professor of chemistry at Florida Gulf Coast University, where he performs research in computational chemistry with applications to environmental, materials, and biological/medicinal chemistry.

SoFL-ACS Executive Committee Meeting

2 – 4 PM, Friday, January 20, 225A Whitaker Hall, Florida Gulf Coast University, Ft. Myers. All SoFL-ACS members welcome.

2023 SoFL-ACS Officers

Chair – Thomas K. (T.K.) Harris, University of Miami, 305-243-3358,

tharris@miami.edu

Chair-Elect – Marc Knecht, University of Miami, 305-284-9351,

knecht@miami.edu

Past Chair – John Reilly, Florida Gulf Coast University, 239-590-1881,

johnreilly@fgcu.edu

Secretary and Councilor – Milagros Delgado, FIU-BBC, 305-919-5966,

degadom@fiu.edu

Treasurer – Jesse Bernstein, 440-821-4623, Jbern0309@gmail.com

Councilor – George Fisher, 954-870-8458; gfisher@barry.edu

Councilor – Zaida Morales-Martinez, 305-386-3206, moralesz@fiu.edu

Alternate Councilor – Jesse Bernstein, 440-821-4623, Jbern0309@gmail.com

Alternate Councilor – Lisa Milenkovic, 754-321-2119,

lisa.milenkovic@browardsschools.com

Alternate Councilor – Vic Shanbhag, Nova Southeastern Univ. 954-262-3931,

shanbhag@nova.edu