



The Orange County Section of the American Chemical Society

February Dinner Meeting
Thursday, February 20, 2019

The Doubletree Club Hotel
7 Hutton Centre Drive, Santa Ana
Phone: 714-751-2400

Social: 5:30PM
Dinner: 6:00PM
Presentation: 7:20PM

**Computational Investigations into the
Mechanism of Sulfur (VI) Fluoride Activation**

Maduka Ogba

Assistant Professor of Chemistry, Chapman University, Orange

Reservations

Please email OCACS@sbcglobal.net ASAP but no later than **12 noon** on **Monday, February 18, 2019**. Indicate if you will be attending the dinner and program or the program only, and list the names of all attendees. Dinner cost is \$30 for members and members' significant others; \$35 for non-members or those without reservations. Pay in cash or by check at the door, or mail a check in advance to OCACS, P.O. Box 211, Placentia CA 90871. **The first five students who register for a meeting will receive a \$10 discount on their dinner.**

There is no charge for attending the program only. However, voluntary donations will be accepted to help defray meeting costs.

Note: OCACS pays the hotel on the basis of the number of dinner reservations made. Your RSVP for dinner is a commitment to pay for dinner. Space may be limited.

Directions

Take the Costa Mesa Freeway (55), exit at MacArthur Blvd. and go west (towards South Coast Plaza). Turn left on to MacArthur Place. The DoubleTree *Club* Hotel is straight ahead on the left. (Do not turn right at MacArthur Place to the DoubleTree Hotel, which is easily mistaken for the DoubleTree Club Hotel.) Park in front of the hotel, or follow the signs. If the parking lot is full, ask the valet staff where to park.

Computational Investigations into the Mechanism of Sulfur (VI) Fluoride Activation

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Abstract

Sulfur-Fluorine Exchange (SuFEx) chemistry is emerging as a promising type of click-chemistry to convert sulfur (VI) fluorides into a variety of sulfonylated compounds. Sulfur (VI) fluorides are particularly attractive compared to their chloride analogs due to the increased resistance to reduction, thermodynamic stability, and chemoselectivity. A key requirement for successful SuFEx chemistry is in the development of conditions conducive for activating the strong sulfur (VI) fluoride S-F bond. However, detailed exploration into the modes of S(VI)-F bond activation is in its infancy. In this talk, insights from computations into the activation of sulfur (VI) fluorides will be discussed.

Biography

Maduka joined the Chemistry and Biochemistry faculty at Chapman University in 2018. He conducted his Ph.D. at Oregon State with Prof. Paul Cheong, and his Robbins Postdoctoral Fellowship at Pomona College with Prof. Dan O'Leary. His research group at Chapman is invested in using computational techniques to unravel the underlying physical and chemical interactions governing molecular structure, reaction mechanisms, and selectivity in organocatalyzed reactions.