Tuesday, July 01, 2025 (2pm-4pm, IEM Conference Room)

Decoding Surface Chemistry for Advanced ROS-Generating Materials

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Reactive oxygen species (ROS) are highly reactive oxygen-derived molecules that play a crucial role in photocatalytic processes, including water treatment and pollutant degradation, due to their strong oxidative properties. Additionally, ROS can induce oxidative damage to cellular components, leading to potential biological applications such as antibacterial, antifungal, and antiviral effects.

In this work, we present recent efforts from our research group to elucidate the physicochemical mechanisms governing ROS formation on silver-based metal oxide surfaces. We start showing key issues in the structural properties of these materials aided by atomistic ab initio thermodynamics approaches. We also present density functional theory (DFT) calculations and ab initio molecular dynamics (AIMD) simulations, which provide valuable insights into the activation of oxygen and water molecules, shedding light on key factors that drive ROS generation.

References:

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Miguel A. San-Miguel is an Associate Professor at the State University of Campinas (Unicamp), Brazil, where he has been a faculty member since 2014 and currently serves as Head of the Physical Chemistry Department. He leads the Unicamp Materials Simulation Lab (UMSL). He earned his Ph.D. in Chemistry from the Universidad de Sevilla (Spain) in 1998, where he later held a faculty position as Associate Professor in Physical Chemistry until 2014. He conducted postdoctoral research at the Universities of Reading and Warwick (UK), and was a Visiting Professor at the University of Oxford (UK) from 2008 to 2009.

His research focuses on atomistic computer modeling of functional materials for catalysis, biomaterials, and related applications. Using DFT-based methods and classical simulations, his group investigates the fundamental physicochemical processes at the atomic scale that underpin materials performance. Research efforts are conducted in close collaboration with experimental groups, fostering integrated insights and advancing scientific knowledge.