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Rapid Screening Of Single Metal Atom Catalysts Supported On Titania For The Decomposition Of Chemical Warfare Agent Using Density Functional Theory

Celine Tesvara University of California, Los Angeles **Philippe Sautet** University of California, Los Angeles

GB, a toxic nerve agent, continues to be one of the primary choices for terrorists in conducting attacks. Recent research has highlighted the efficacy of single-atom catalysts (SAC) supported on metal oxides in promoting oxidation reactions. Concurrently, metal oxides have been observed to exhibit strong interactions with GB/DMMP. Leveraging Density Functional Theory (DFT), this study delves into the respective roles of SAC and metal oxides in the decomposition of GB & DMMP. The investigation begins with an exploration of GB and DMMP binding modes with Pt1/a-TiO2(101), revealing key difference in DMMP's ability to adopt.

The authors acknowledge support from the U.S. Army under Program No. W911NF-21-1-0361. This work uses computational resources hosted by the Hoffman2 Shared Cluster provided by UCLA and by the Bridges-2 at Pittsburgh Supercomputing Center through allocation CHE170060 from the Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) program, which is supported by NSF grants #2138259, #2138286, #2138307, #2137603, and #2138296.