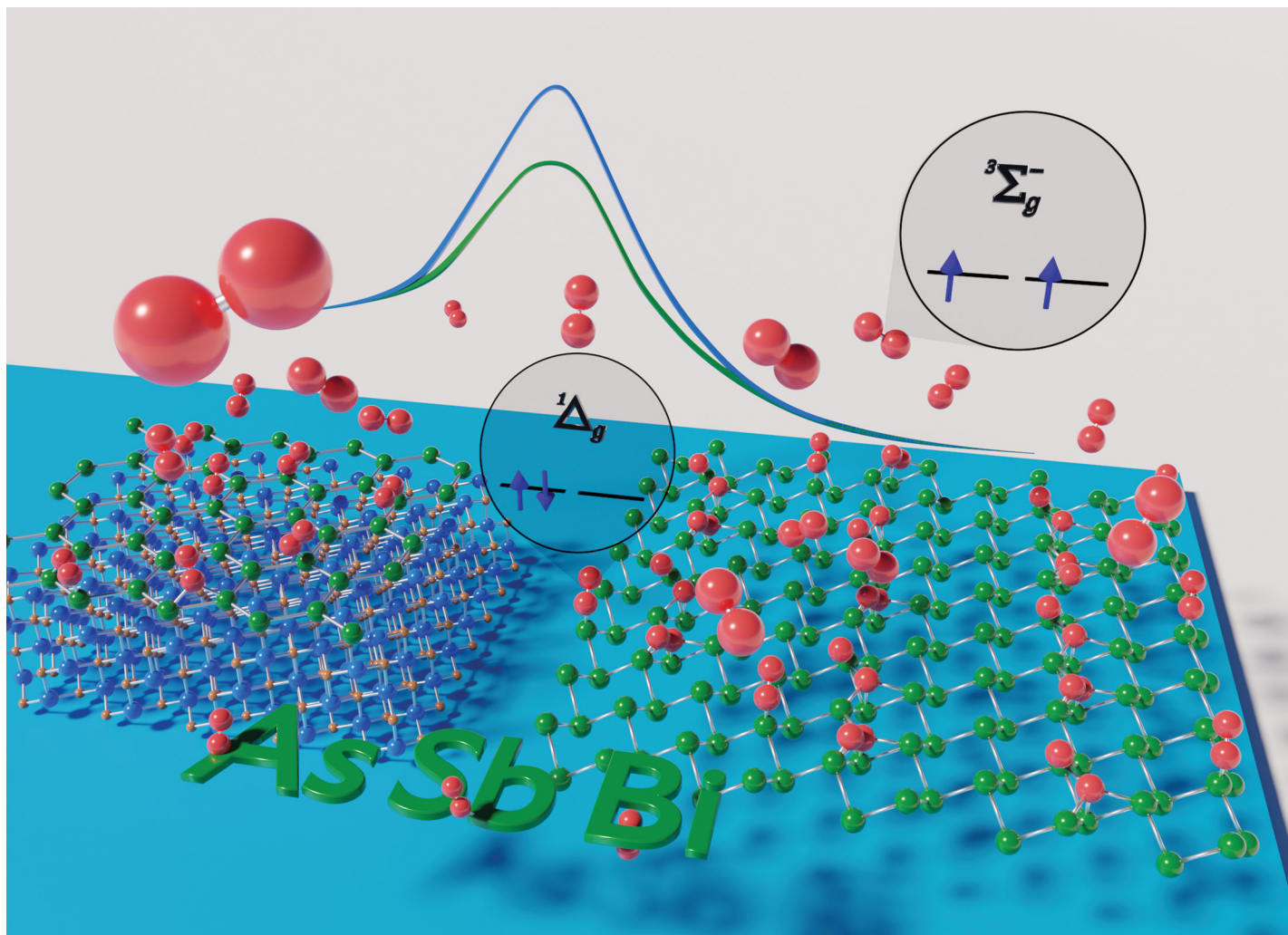




Showcasing research from the Group of Prof. Adalberto Fazzio at the Brazilian Center for Research in Energy and Materials, Brazil

Substrate suppression of oxidation process in pnictogen monolayers

Oxidation process control is challenging in experimental conditions. Through *ab initio* calculations, we investigated the O₂ molecule interaction with two-dimensional (2D) mono-elemental materials from the pnictogen family in the freestanding and substrate-supported cases. Besides, we evaluated the role of O₂ multiplets and spin-orbit coupling (SOC) effects within the oxidation mechanisms. Substrate and SOC effects are crucial, affecting reaction energy barriers and oxidation time scales. Our study will bring valuable insights into the experimental realization of 2D materials in environmental conditions.

As featured in:



See F. Crasto de Lima *et al.*, *Phys. Chem. Chem. Phys.*, 2024, **26**, 9149.