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Theoretical Insights into CO_2 Activation on α-Bi_2O_3 under Operating Conditions

Theoretical Insights into CO_2 Activation on α-Bi_2O_3 under Operating Conditions

The increasing use of fossil fuels over recent decades has triggered a global energy crisis, marked by the rapid depletion of these resources and the substantial release of carbon dioxide (CO_2) into the atmosphere [1]. CO_2 levels are projected to reach 570 ppm by 2100, a rise that contributes to critical environmental challenges such as global warming, polar ice melt, and ocean acidification [2]. To mitigate these effects and move toward a carbon-neutral cycle, strategies that utilize CO_2 as a feedstock for producing value-added chemicals have become increasingly important. Among these, the electrochemical CO_2 reduction reaction (CO_2RR) has emerged as a promising approach for CO_2 conversion under mild conditions. However, several challenges need to be addressed: CO_2 activation is energy-demanding due to its high thermodynamic stability, CO2 conversion efficiency is generally limited by the competing Hydrogen Evolution Reaction (HER), and the selectivity towards specific products is low [3]. In recent years, bismuth-based electrocatalysts have gained much attention owing to their low toxicity, cost-effectiveness, abundance, and high selectivity for CO_2 conversion to formate or formic acid via electrochemical CO_2RR [4–6]. Nonetheless, achieving substantial progress requires a deeper microscopic understanding of the underlying processes. Due to their explicative and predictive power, ab initio calculations play a key role in the energy scenario as they characterize from an atomistic perspective the complex materials and give insights into the catalytic mechanisms. Previous computational studies on CO_2RR on Bi_2O_3 have focused on pristine and defective surfaces [6], or the influence of decorating metallic nanocluster (NC) [7]. In this work, we extend these efforts by investigating the thermodynamically stable α-phase of Bi_2O_3 as a potential electrocatalyst for CO_2RR, taking into account the impact of oxygen vacancies and the role of an externally applied bias (i.e., operating electrochemical conditions) [8].

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Primary author(s) : Ms. D'ANANIA, Olga (Scuola Superiore Meridionale); Dr. FASULO, Francesca (Università degli studi di Napoli Federico II); Prof. PAVONE, Michele (Università degli Studi di Napoli Federico II); Prof. TALARICO, Giovanni (Università degli Studi di Napoli Federico II); Prof. MUÑOZ-GARCÍA, Ana B. (Università degli Studi di Napoli Federico II)

Presenter(s) : Ms. D'ANANIA, Olga (Scuola Superiore Meridionale)