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Single-Atom Catalysts on Goldene

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In single-atom catalysis, the interaction between isolated metal atoms and the supporting matrix plays a pivotal role in determining the stability and reactivity of the system. This has driven the search for novel supporting materials, particularly 2D materials, where graphene has been the predominant choice. Simultaneously, increasing attention is being given to Single-Atom Alloys (SAAs)[1], a subclass of Single-Atom Catalysts (SACs) where the supporting matrix is a metal itself. Recently, Kashiwaya et al.[2] reported the synthesis of goldene, a self-standing 2D monolayer of Au(111) described as the gold analogue of graphene. Motivated by this breakthrough, we explored a new class of SACs consisting of transition metal (TM) atoms stabilized on goldene. The atomistic nature of Au-ene requires simulations, where we rely on VASP with a PBE+U functional.[3,4] Through electronic structure calculations, we identified several systems that remain stable under both reducing and oxidizing conditions.[5] We then investigated their catalytic performance in the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), discovering that certain TM-goldene systems exhibit promising activity, with reactivity significantly different from the same TMs supported on bulk Au(111). Our analysis included a comprehensive evaluation of potential reaction intermediates, extending beyond the conventional species typically assumed in HER and OER.[6] This study provides strong theoretical evidence that SACs embedded in goldene could offer promising stability and catalytic reactivity.

[1] Single-Atom Alloy Catalysis, R. T. Hannagan, G. Giannakakis, M. Flytzani-Stephanopoulos, E. C. H. Sykes, American Chemical Society, 2020, DOI: 10.1021/acs.chemrev.0c00078. [2] S. Kashiwaya, Y. Shi, J. Lu, D. G. Sangiovanni, G. Greczynski, M. Magnuson, M. Andersson, J. Rosen, L. Hultman, Nature Synthesis 2024, 3, 744, DOI: 10.1038/s44160-024-00518-4. [3] C. Saetta, I. Barlocco, G. Di Liberto, G. Pacchioni, Small 2024, 20, 2401058, DOI: https://doi.org/10.1002/smll.202401058. [4] G. Di Liberto, G. Pacchioni, Advanced Materials 2023, 35, 2307150, DOI: https://doi.org/10.1002/adma.202307150. [5] G. Di Liberto, L. Giordano, G. Pacchioni, ACS Catal 2024, 14, 45, DOI: 10.1021/acscatal.3c04801. [6] I. Barlocco, L. A. Cipriano, G. Di Liberto, G. Pacchioni, J Catal 2023, 417, 351, DOI: 10.1016/j.jcat.2022.12.014.

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