Scientists reveal synergistic effects in dual single-atom catalyst

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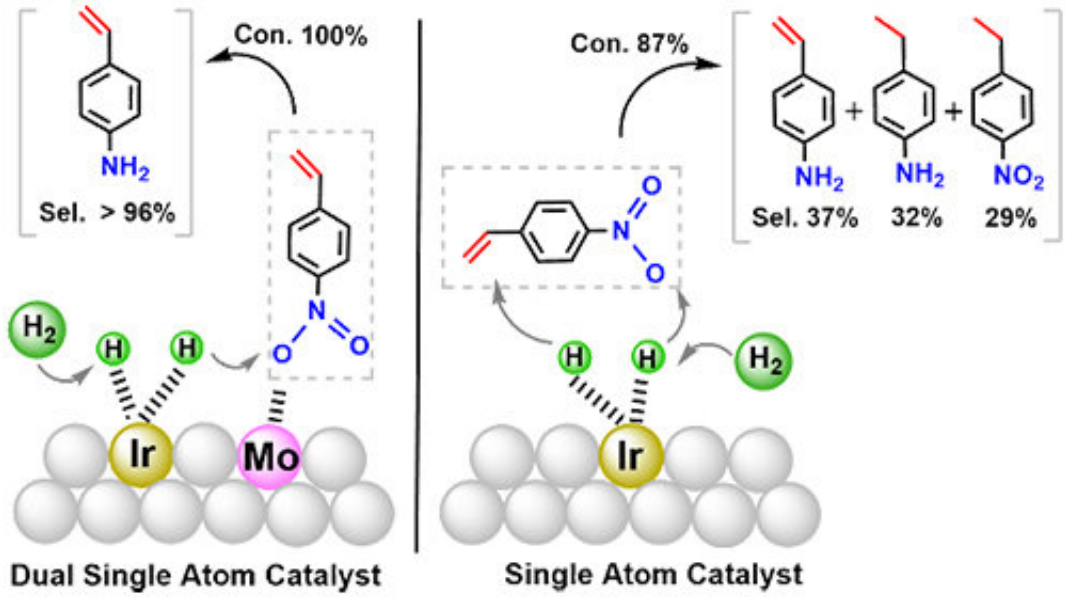

Synergistic effects for enhanced catalysis in a dual single-atom catalyst. Credit: FU Junhong

Single-atom catalysts (SACs) are applied in heterogeneous catalysis. Instead of one type of single atom, dual single-atom catalysts (DSACs) deliver superior catalytic performance than SACs due to cooperation between the dual metal-atoms.

Understanding synergistic effects at the atomic scale is critical for the design of highly effective heterogeneous catalysts in chemical

transformation.

Recently, Prof. Huang Jiahui's group and Prof. Fu Qiang's group from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS), in cooperation with Prof. Si Rui from Shanghai Institute of Applied Physics, CAS, revealed synergistic catalysis of dual single-atom structure in the selective hydrogenation 4-nitrostyrene (4-NS) to 4-vinylaniline (4-VA).

The study was published in *ACS Catalysis* on Jan. 29.

The researchers synthesized DSAC Ir_1Mo_1/TiO_2 as well as SACs Ir_1/TiO_2 and Mo_1/TiO_2. They found that DSAC Ir_1Mo_1/TiO_2 displayed a superior catalytic performance for selective hydrogenation of 4-NS to 4-VA than SACs Ir_1/TiO_2 and Mo_1/TiO_2.

Computational results indicated that H_2 activation occurred on Ir_1 and 4-NS adsorption via the nitro group preferentially occurred on Mo_1, with the synergistic effect of Ir_1 and Mo_1 leading to enhanced catalytic performance.

This work elucidates the atomic level advantages of DSAC in promoting reaction mechanisms for efficient heterogeneous bimetallic catalysis.

More information: Junhong Fu et al. Synergistic Effects for Enhanced Catalysis in a Dual Single-Atom Catalyst, *ACS Catalysis* (2021). DOI: 10.1021/acscatal.0c05599

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