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\textsubscript{1}Mo\textsubscript{1}/TiO\textsubscript{2} as well as SACs Ir\textsubscript{1}/TiO\textsubscript{2} and Mo\textsubscript{1}/TiO\textsubscript{2}. They found that DSAC Ir\textsubscript{1}Mo\textsubscript{1}/TiO\textsubscript{2} displayed a superior catalytic performance for selective hydrogenation of 4-NS to 4-VA than SACs Ir\textsubscript{1}/TiO\textsubscript{2} and Mo\textsubscript{1}/TiO\textsubscript{2}.

Computational results indicated that H\textsubscript{2} activation occurred on Ir\textsubscript{1} and 4-NS adsorption via the nitro group preferentially occurred on Mo\textsubscript{1}, with the synergistic effect of Ir\textsubscript{1} and Mo\textsubscript{1} leading to enhanced catalytic performance.

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


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