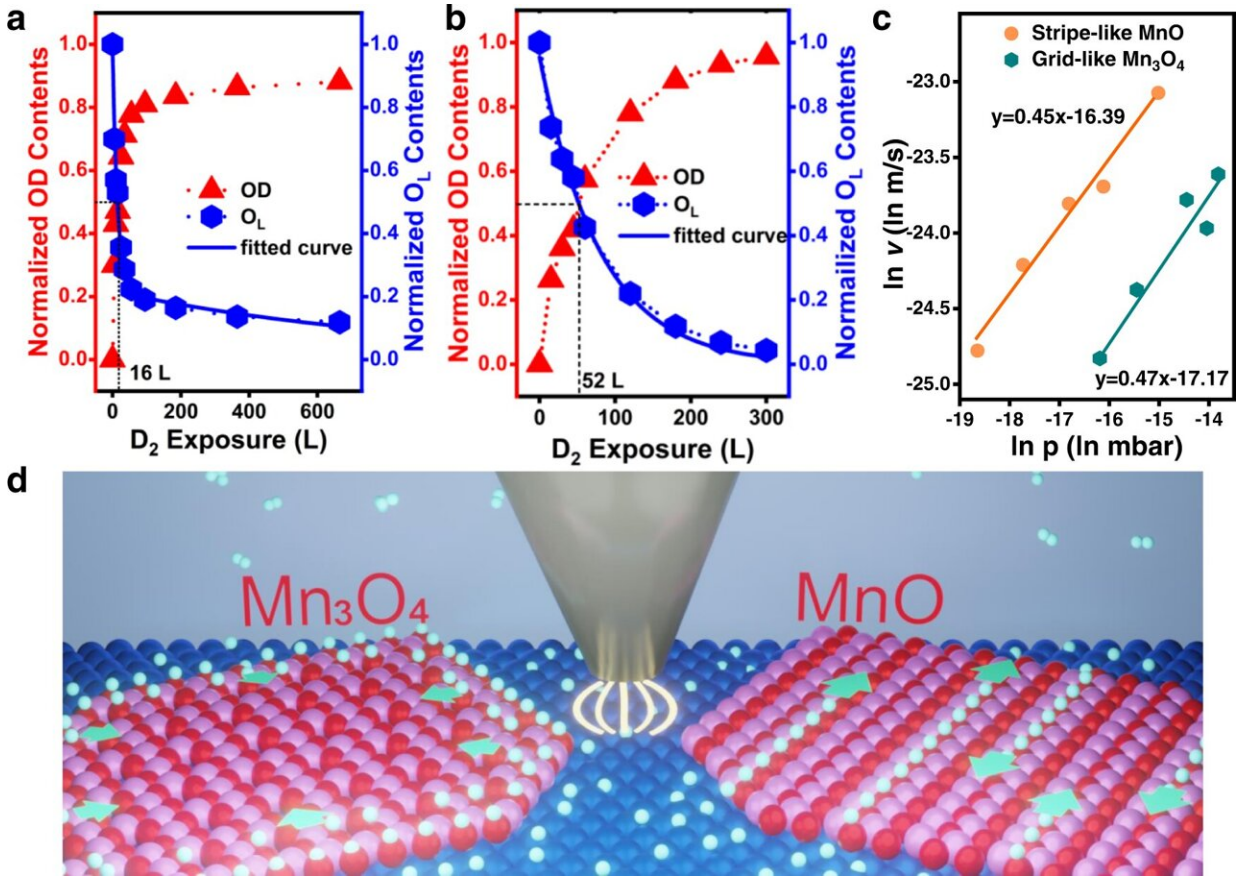
Surface-lattice-confinement effect accelerates hydrogen spillover

February 8 2023, by Li Yuan



Hydrogen spillover rates on MnO and Mn_3O_4. OD and O_L contents derived from the XPS O 1s areas of (a) stripe-like MnO and (b) grid-like Mn_3O_4 surfaces with different amount of D_2 exposure. c Dependence of spillover rates of stripe-like MnO and grid-like Mn_3O_4 surfaces on H_2 partial pressure. The logarithms of spillover rates vs. logarithms of p_{H2}. d Schematic of HP-STM using a STM tip to probe the hydrogen spillover on MnO and Mn_3O_4 surfaces in H_2 atmosphere. Pt: dark blue; Mn: light violet; O: red; H: cyan. Credit: *Nature Communications*

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Hydrogen spillover is the dynamic migration of surface-adsorbed hydrogen species from hydrogen-rich sites to hydrogen-poor sites. It plays an important role in many H-involving reaction processes.

In order to enhance the catalytic performance of H-involving reactions, it is important to understand the detailed mechanism of hydrogen spillover and learn how hydrogen transfers and what factors control hydrogen conductivity on solid surfaces.

Recently, a research team led by Prof. Mu Rentao and Prof. Fu Qiang from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS) directly observed the acceleration of hydrogen spillover via a surface-lattice-confinement effect.

This work was published in *Nature Communications* on Feb. 4.

The researchers constructed stripe-like MnO(001) and grid-like $Mn3O_4$(001) monolayers on a Pt(111) substrate, and investigated their hydrogen spillover.

They found that hydrogen species from Pt diffused unidirectionally along the stripes on MnO(001), whereas it exhibited an isotropic pathway on Mn_3O_4(001).

Moreover, by using dynamic surface imaging in an H_2 atmosphere, they revealed that hydrogen diffused four times more rapidly on MnO than was the case on $Mn3O_4$, which was promoted by a one-dimension surface-lattice-confinement effect.

Theoretical calculations indicated that a uniform and medium O-O distance favored hydrogen diffusion while low-coordinate surface O atom inhibited it.

"Our study illustrates the surface-lattice-confinement effect of oxide catalysts on hydrogen spillover and provides a promising route to improve the hydrogen spillover efficiency," said Prof. Fu.

More information: Yijing Liu et al, Direct observation of accelerating hydrogen spillover via surface-lattice-confinement effect, *Nature Communications* (2023). DOI: 10.1038/s41467-023-36044-8

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