Researchers discover C-H bond activation reactions at low temperature by photo-induced means

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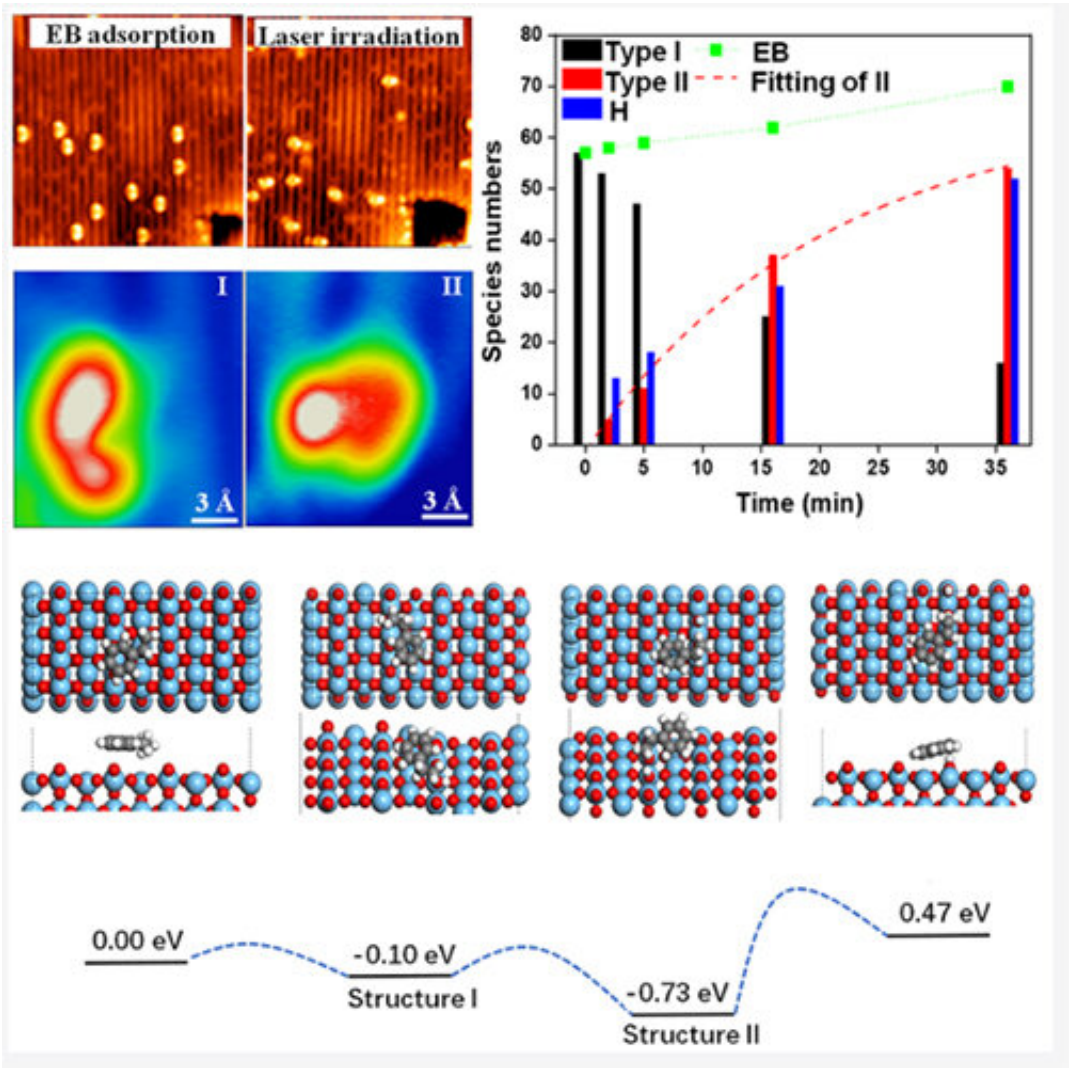

High-resolution STM visualizing the intermediate states of the reaction and the reaction pathway of EB dehydrogenation on TiO2. Credit: WANG Haochen

The C-H bond is very important in organic chemistry. Chemical reactions related to the breaking and further synthesis of the C-H bond require high activation energy and poor selectivity. Therefore, it's important to understand the reaction mechanism of the C-H bond.

Recently, a research team led by Prof. Yang Xueming and Prof. Ma Zhibo from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS), in collaboration with Prof. Pan Minghu from the Huazhong University of Science and Technology, discovered the C-H bond breaking reaction catalyzed by low-temperature photocatalysis on the surface of titanium oxide, and explained the reaction mechanism at the single molecule level.

The results were published in the *Journal of Physical Chemistry Letters* on Nov. 10.

The scientists used the rutile 110 surface of titanium oxide as the model system and the C-H bond molecule ethylbenzene as the model molecule.

They found that ethylbenzene could be induced to remove hydrogen at low temperature (77K) only by photoinduced reaction. They also experimentally observed the images of the reaction steps by in-situ tracking single molecules.

Prof. Pan's team provided support for the theoretical interpretation of the image and confirmed the reaction process.

More information: Haiping Lin et al. In Situ Observation of Stepwise C–H Bond Scission: Deciphering the Catalytic Selectivity of Ethylbenzene-to-Styrene Conversion on TiO_2, *The Journal of Physical Chemistry Letters* (2020). DOI: 10.1021/acs.jpclett.0c02729