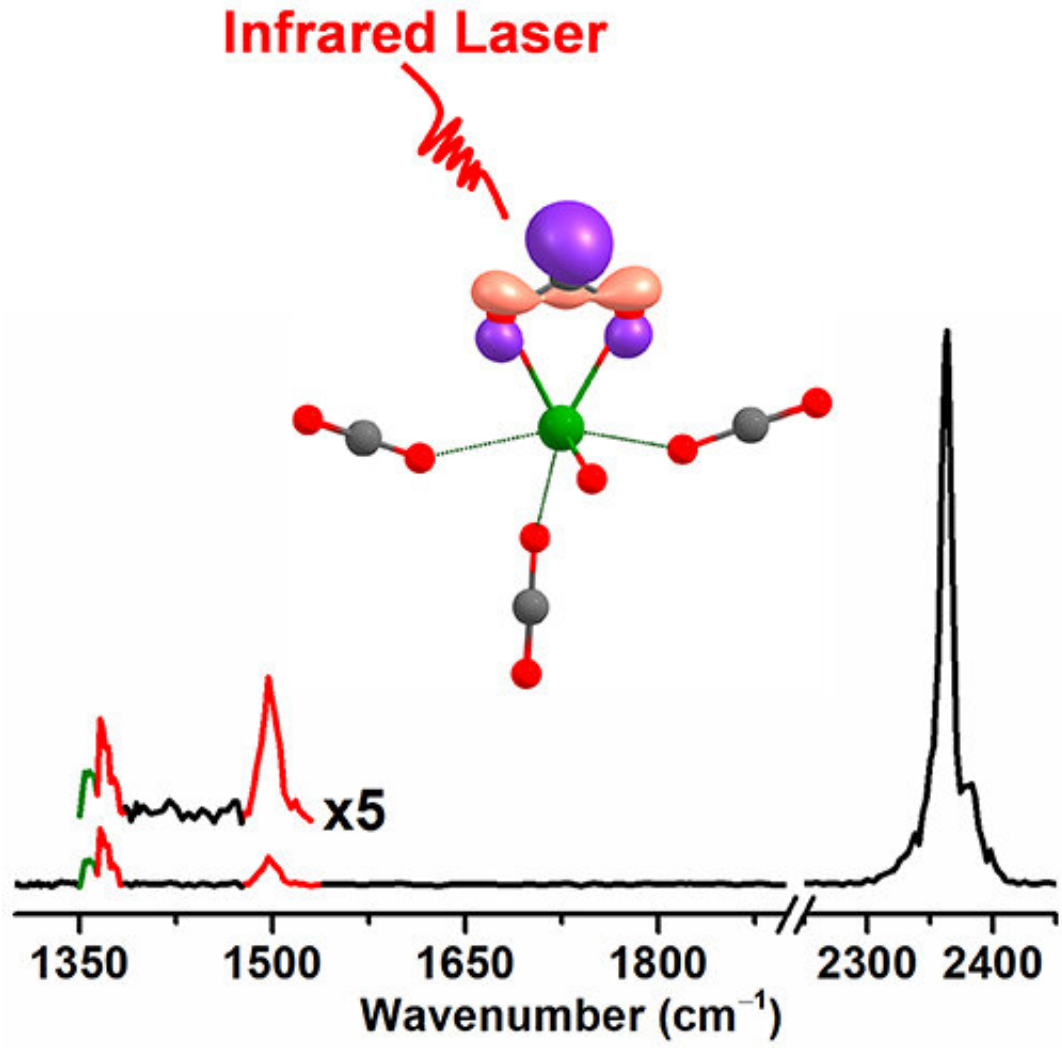
Scientists identify transition metal for highly-efficient carbon dioxide activation

January 5 2021, by Li Yuan



Spectroscopic identification of transition-metal M[η^2-(O,O)C] species for highly-efficient CO2 activation. Credit: ZHENG Huijun

The atmospheric concentration of carbon dioxide (CO_2) has been increasing over the past century, imposing severe consequences for global climate change and planetary temperature increase.

To reduce CO_2 from the atmosphere and take it as the feedstock for sustainable energy sources, the capture and utilization of CO_2 to create valuable chemicals is highly desired.

A research team led by Prof. Jiang Ling and Prof. Fan Hongjun from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences, in collaboration with Prof. Zhao Zhi from Hebei University of Engineering, characterized a transition metal M[η2-(O,O)C] species for highly-efficient CO_2 activation.

The result was published in the *Journal of Physical Chemistry Letters* on Dec. 28.

Based on the recently-developed infrared photodissociation spectroscopy apparatus, the researchers synthesized and characterized an unprecedented transition metal M[η2-(O,O)C] motif with bidentate double oxygen metal-CO_2 coordination in the $[ZrO(CO_2)n>=4]^+$ complexes.

The Zr[η2-(O,O)C] species yielded a CO_2- radical ligand, showing high efficiency in CO_2 activation. The CO_2^- radical and non-linear character of these series of M[η^2-(O,O)C] complexes might enable high reactivity in many important reactions such as C-C coupling and C-H activation.

There were two important prerequisites for certain metals to form this intriguing M[η^2-(O,O)C] species: the metal center had high reduction capability and the oxidation state of the metal center was lower than its highest one by one.

Systematic analyses for the effects of different transition and main-group metals on the formation of M[η^2-(O,O)C] complexes provided comprehensive insights into the microscopic mechanism of CO_2 activation by a single metal center, offering design criteria for single-atom catalyst with isolated transition metal atoms dispersed on supports. Such advances might be integrated into the CO_2-activation and -utilization technology.

This study highlights the pivotal roles played by the M[η^2-(O,O)C] species in CO_2 activation and opens new avenues towards the development of related single-atom catalysts with isolated transition metal atoms dispersed on supports.

More information: Huijun Zheng et al. Spectroscopic Identification of Transition-Metal M[η2-(O,O)C] Species for Highly-Efficient CO2 Activation, *The Journal of Physical Chemistry Letters* (2020). DOI: 10.1021/acs.jpclett.0c03379

Provided by Chinese Academy of Sciences