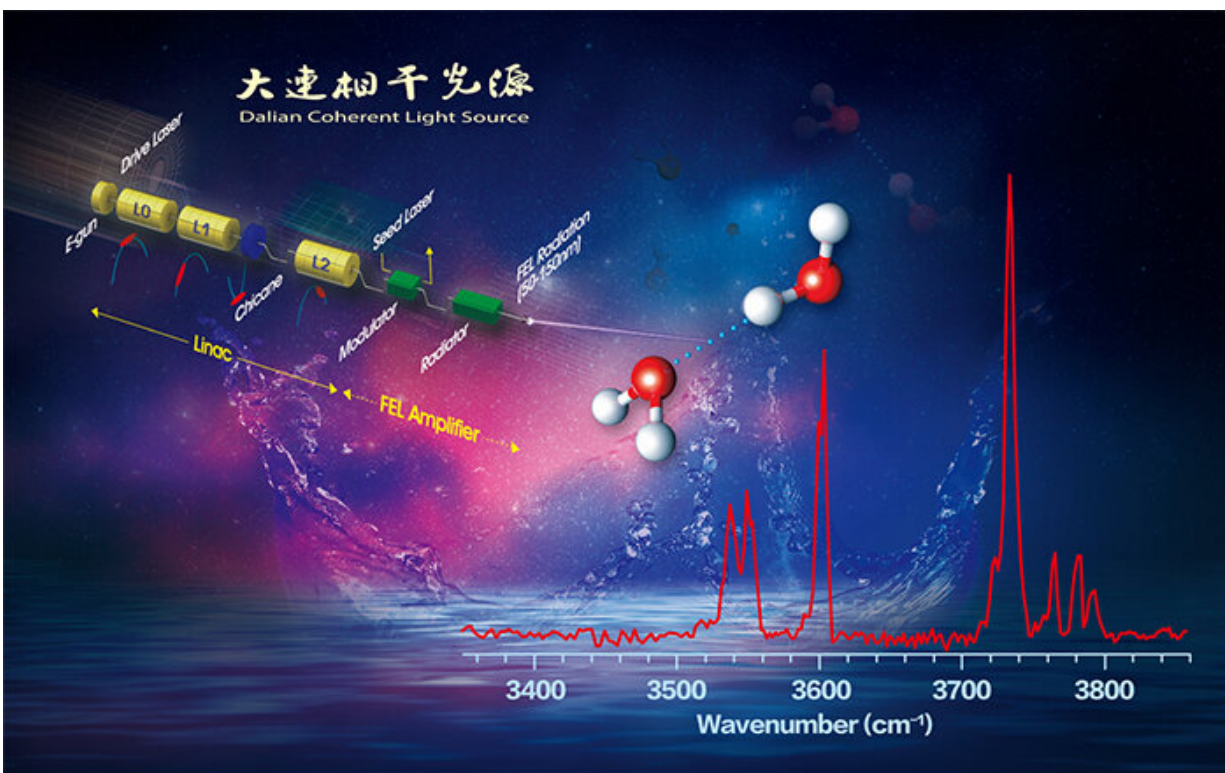


Scientists reveal infrared spectroscopy of neutral water dimer

February 24 2020, by Li Yuan



Infrared spectroscopy of neutral water dimer based on a tunable vacuum ultraviolet free electron laser. Credit: JIANG Ling

A research team led by Profs. Jiang Ling, Yang Xueming and Zhang Donghui from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences, in collaboration with Prof. Li Jun from

Tsinghua University, revealed infrared spectroscopy of neutral water dimer based on a tunable vacuum ultraviolet free electron laser.

Their findings, published in *The Journal of Physical Chemistry Letters*, help to resolve the controversy of the exact vibrational assignment of each band feature of water dimer.

Optical [spectroscopy](#) of gas-phase clusters provides detailed structural and dynamical information. Easy size-selection and detection can be realized in the spectroscopic study of charged clusters; while neutral clusters face challenges due to the absence of a charge.

Based on the VUV Free Electron Laser (FEL) delivered by Dalian Coherent Light Source (DCLS), the research team built an infrared (IR)-VUV spectroscopy apparatus and successfully measured the IR spectra of the water dimer.

Since clusters with different sizes have different ionization energies, the tunable VUV-FEL light paves the way for selectively ionizing a given neutral [cluster](#) free of confinement, thus facilitating realization of their size selectivity. This unique VUV-FEL facility makes it possible to study the IR spectroscopy of confinement-free, neutral clusters via the IR-VUV scheme.

The electronic structure analyses are helpful for understanding the spectroscopic features of OH vibrational modes for different hydrogen bond orientation in more complicated water clusters.

As many clusters have their ionization energies in a range accessible by VUV-FEL light source and near threshold ionization can be readily achieved, the VUV-FEL based IR spectroscopy opens a new paradigm for the study of vibrational spectra of a wide variety of neutral clusters.

The availability of these new experimental data on the neutral clusters is expected to stimulate further calculations and development of theoretical methods, leading to an improved understanding of the structures and dynamics of these systems.

More information: Bingbing Zhang et al. Infrared Spectroscopy of Neutral Water Dimer Based on a Tunable Vacuum Ultraviolet Free Electron Laser, *The Journal of Physical Chemistry Letters* (2020). [DOI: 10.1021/acs.jpcllett.9b03683](https://doi.org/10.1021/acs.jpcllett.9b03683)

Provided by Chinese Academy of Sciences

Citation: Scientists reveal infrared spectroscopy of neutral water dimer (2020, February 24)
retrieved 2 May 2024 from
<https://phys.org/news/2020-02-scientists-reveal-infrared-spectroscopy-neutral.html>

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