ISSN 0567-7351
CN 31-1320/O6
CODEN HHHPA4
http://sioc-journal.cn

化 学 学 报

ACTA CHIMICA SINICA

Volume 80 Number 5 May 2022

QK2228099

ISSN 0567-7351
05>
770567 735226

万方数据

中国化学会
中国科学院上海有机化学研究所 主办

化 学 学 报

Acta Chimica Sinica

(Huaxue Xuebao)

第 80 卷　第 5 期　2022 年 5 月 15 日

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* 通信联系人.

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ACTA CHIMICA SINICA

Vol. 80, No. 5 May 15, 2022

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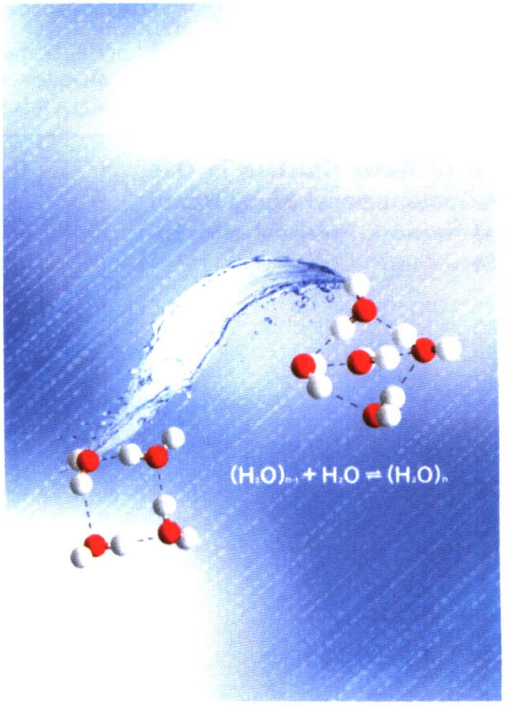
On the cover: A dual post-treatment method is developed by combining surface rinse with ultraviolet-ozone treatment to optimize structures and properties of Mg-doped NiO (NiMgO) semiconductor films. Using the ternary NiMgO films as a novel type of hole transport layers, highly efficient and stable organic solar cells are achieved with a non-fullerene bulk heterojunction of PM6:M36. [Yin, Zhigang *et al.* on page 581-589.]



On the back cover: Monte Carlo simulations with a neural network potential reveal the gas phase nucleation behavior of water molecules. The transition from two-dimensional ring structures to three dimensional hydrogen bond network structures starts at $(H_2O)_5$ although the ground-state structure of $(H_2O)_5$ remains to be a two-dimensional ring. [Li, Zhenyu *et al.* on page 598-606.]

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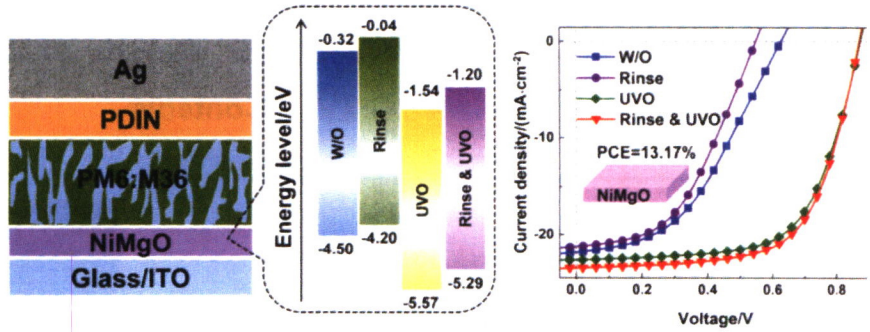
Article

A Dual Post-Treatment Method for Improving the Performance of Ternary NiMgO Semiconductor Interfacial Layers and Their Organic Solar Cells

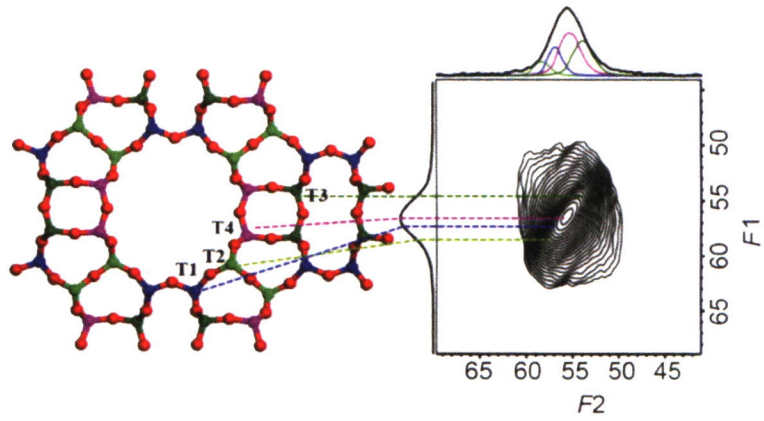


A new dual post-treatment method is designed by combining surface rinse with ultraviolet-ozone (UVO) treatment to optimize structures and properties of NiMgO films for photovoltaic applications. Benefiting from the improved energy level alignment, increased transmittance and smoothed surface of NiMgO as a novel hole transport layer derived from the dual post-treatment, the resulted non-fullerene organic solar cells deliver highly improved efficiencies from 5.90% to 13.17%.

He, Xinrui; Cai, Lina; Chen, Hansheng; Yin, Pan; Yin, Zhigang*; Zheng, Qingdong*

Acta Chim. Sinica **2022**, *80*(5), 581-589

Study on the Framework Aluminum Distributions of HMOR Zeolite and Identification of Active Sites for Dimethyl Ether Carbonylation Reaction

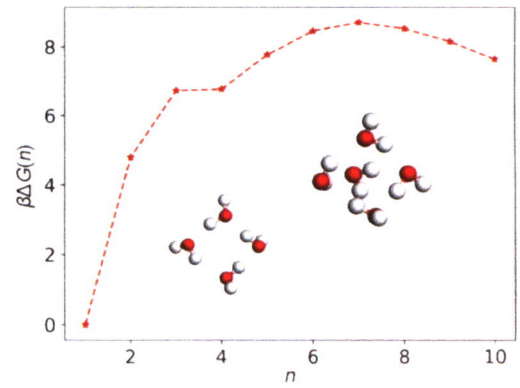


The framework Al sites of MOR zeolite has been distinguished by 2D ^{27}Al multiple-quantum magic angle spinning nuclear magnetic resonance (MQ MAS NMR) technique that illuminates the active site for dimethyl ether carbonylation reaction.

Zhang, Jin; Ding, Xiangnong; Liu, Hongchao; Fan, Dong; Xu, Shutao*; Wei, Yingxu; Liu, Zhongmin

Acta Chim. Sinica **2022**, *80*(5), 590-597

Nucleation of Water Clusters in Gas Phase: A Computational Study Based on Neural Network Potential and Enhanced Sampling



Monte Carlo simulations with a neural network potential reveal the gas phase nucleation behavior of water molecules. A transition from two-dimensional ring structures to three-dimensional hydrogen bond network structures starts when the cluster size increases from 4 to 5, although the ground-state structure of $(H_2O)_5$ remains to be a two-dimensional ring.

Xu, Sen; Wu, Liling; Li, Zhenyu*

Acta Chim. Sinica **2022**, *80*(5), 598-606

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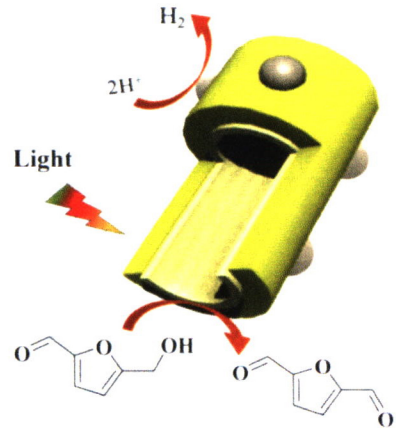
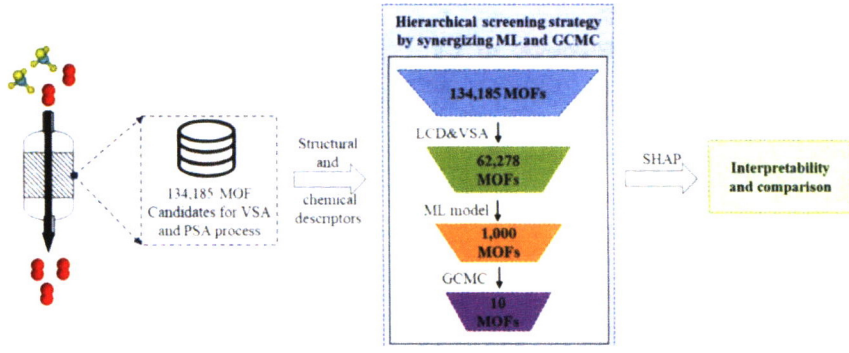
Photocatalytic Oxidation of 5-Hydroxymethylfurfural Selectively into 2,5-Diformylfuran with CdS Nanotube



Shu, Heng; Bao, Yide-Rigen; Na, Yong*

Acta Chim. Sinica **2022**, *80*(5), 607-613

High-Throughput Computational Screening of Metal-Organic Frameworks for CH_4/H_2 Separation by Synergizing Machine Learning and Molecular Simulation

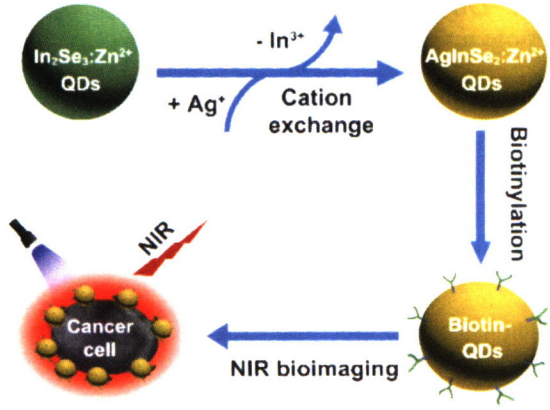


Wang, Shihui; Xue, Xiaoyu; Cheng, Min; Chen, Shaochen; Liu, Chong; Zhou, Li; Bi, Kexin; Ji, Xu*

Acta Chim. Sinica **2022**, *80*(5), 614-624

This work proposed a hierarchical screening strategy by synergizing machine learning and molecular simulation to identify the optimal adsorbents for CH_4/H_2 separation under vacuum swing adsorption and pressure swing adsorption conditions from 134185 hypothetical metal-organic frameworks (MOFs). Interpretability was also provided to explore the transferability potential of the developed model.

Template-Based Controlled Synthesis and Bioapplication of $AgInSe_2:Zn^{2+}$ Near-Infrared Luminescent Quantum Dots



Lian, Wei; Fang, Zekai; Tu, Datao*; Li, Jiayao; Han, Siyuan; Li, Renfu; Shang, Xiaoying; Chen, Xueyuan*

Acta Chim. Sinica **2022**, *80*(5), 625-632

Monodisperse $AgInSe_2:Zn^{2+}$ quantum dots (QDs) with an absolute quantum yield of 42.5% are successfully synthesized via a facile cation exchange strategy from the $In_2Se_3:Zn^{2+}$ template. After biotinylation, these near-infrared luminescent $AgInSe_2:Zn^{2+}$ nanoprobes are employed for targeted cancer cell imaging.

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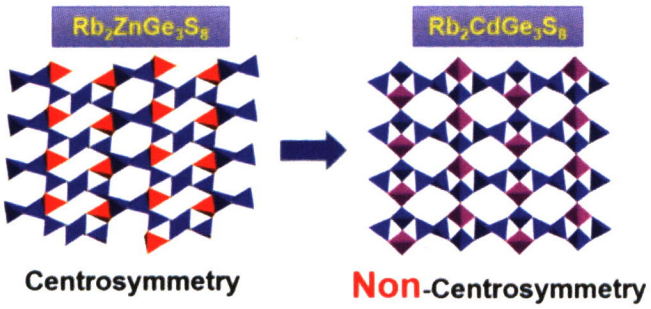
$Rb_2MGe_3S_8$ (M=Zn, Cd): Non-Centrosymmetry Transformation Led by Structure Change of $[MGe_3S_8]^{2-}$ Unit

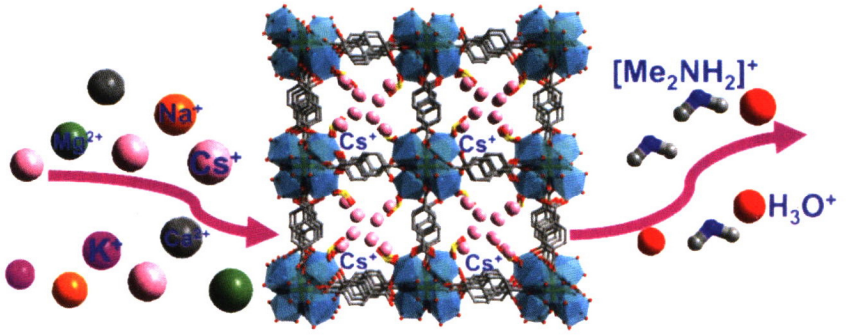


Chai, Xiandan; Chen, Wenfa; Yan, Qiunan; Liu, Binwen; Jiang, Xiaoming*; Guo, Guocong*

Acta Chim. Sinica **2022**, *80*(5), 633-639

By analyzing the basic building units $[MGe_3S_8]^{2-}$ (M=Zn, Cd) of the two chalcogenides, the transition from the centrosymmetry to the non-centrosymmetry was explored. And the theoretical calculations were also performed to deepen our understanding of the origin of nonlinear optical efficiency in $Rb_2CdGe_3S_8$.

Two New Three-Dimensional Lanthanide Metal-organic Frameworks for the Highly Efficient Removal of Cs^+ Ions

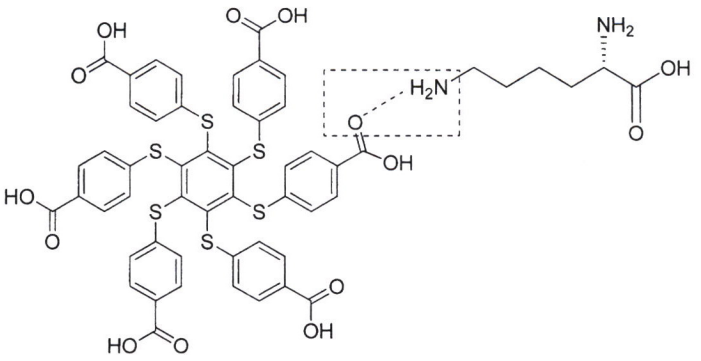


Lü, Tiantian; Ma, Wen; Zhan, Dongsun; Zou, Yanmin; Li, Jilong; Feng, Meiling*; Huang, Xiaoying

Acta Chim. Sinica **2022**, *80*(5), 640-646

The new lanthanide metal-organic frameworks with high water stability can efficiently and selectively remove Cs^+ ions even in the presence of interfering ions. The removal mechanism was elucidated by single-crystal structure analysis and various characterizations attributing to the ion-exchange between Cs^+ ions and $[Me_2NH_2]^+$, $[H_3O]^+$ in the channels.

Circularly Polarized Luminescence and Dynamic Regulation Based on the co-Assembly of *L*/*D*-Lysine Hydrochloride and Photoactivated AIE Molecules



Feng, Xicheng; Zhu, Liangliang; Yue, Bingbing*

Acta Chim. Sinica **2022**, *80*(5), 647-651

The photoactivated aggregation-induced emission (AIE) molecule (M-1) and *L*/*D*-Lysine hydrochloride (*L*/*D*-Lys) co-assemble to form chiral supramolecular *L*/*D*-Lys@M-1 under the action of hydrogen bond, and realize dynamically controllable circularly polarized luminescence (CPL).

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Perspective

Nano-Tracing: Recent Progress in Sourcing Tracing Technology of Nanoparticles

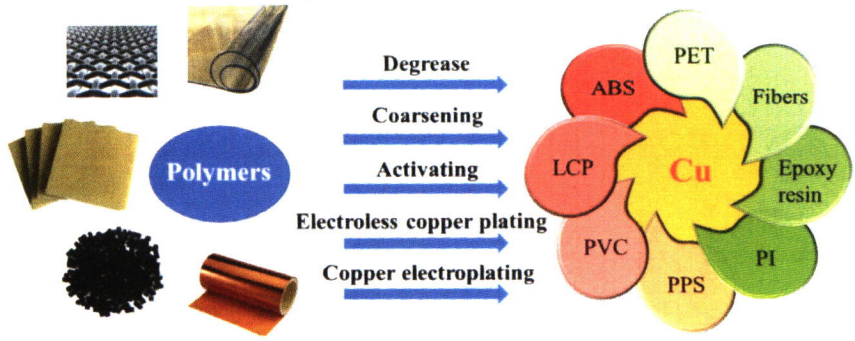
Yang, Xuezhi; Lu, Dawei; Wang, Weichao; Yang, Hang; Liu, Qian*; Jiang, Guibin

Acta Chim. Sinica **2022**, *80*(5), 652-658

Tracing the sources and environmental transformation processes of nanoparticles (NPs) is the prerequisite for their risk assessment and pollution control. The recent progress and the future challenges in the area of source tracing technologies of NPs were reviewed.

Review

Advances in Pretreatments for Electroless Copper Plating on Polymer Materials



Zheng, Anni; Jin, Lei; Yang, Jiaqiang; Li, Weiqing; Wang, Zhaoyun; Yang, Fangzu*; Zhan, Dongping*; Tian, Zhongqun

Acta Chim. Sinica **2022**, *80*(5), 659-667

The properties, compositions and applications of different polymer materials, as well as its pretreatment methods before electroless copper plating have been detailedly overviewed, which can provide guidance for the electroless copper plating on the non-conductive polymer materials' surfaces.

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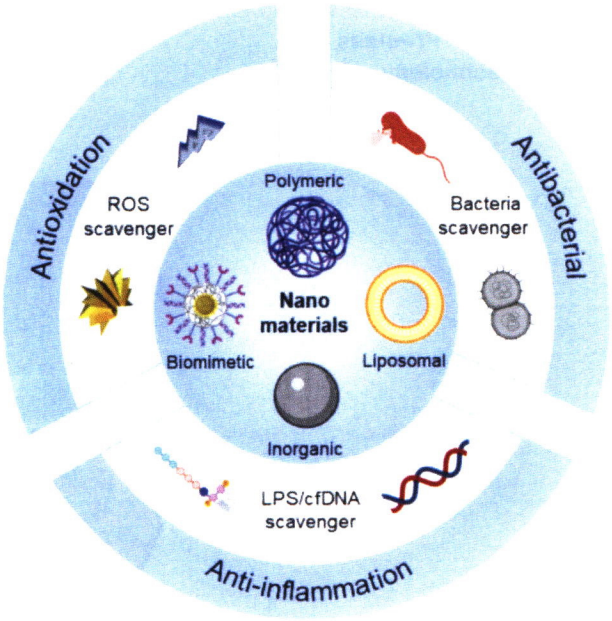
Sepsis Treatment Strategies Based on Nanomaterials

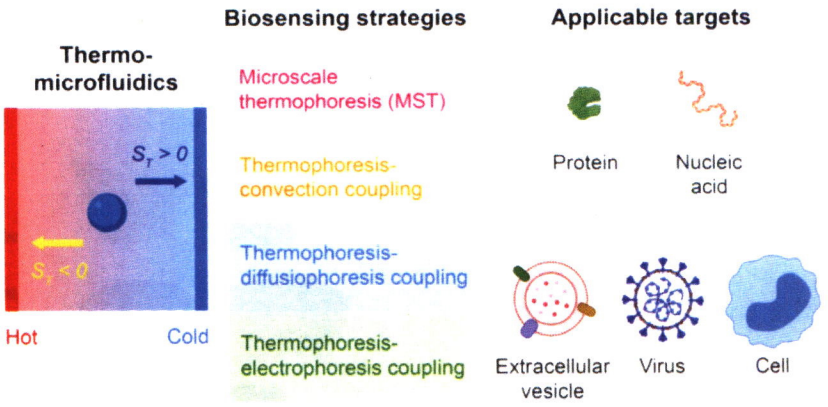


Li, Zhen; Chen, Jie; Tian, Huayu*; Chen, Xuesi

Acta Chim. Sinica **2022**, *80*(5), 668-678

In this review, the latest treatment of sepsis based on nanomaterials is reviewed detailly from various perspectives, including antibacterial, scavenging of reactive oxygen species and dangerous molecules. Then, the problems and challenges facing the treatment of sepsis using nanomaterials are further summarized and discussed. It is anticipated to provide new ideas and solutions for the clinical treatment of sepsis.

Thermomicrofluidic Biosensing Systems



Liu, Chao; Tian, Fei; Deng, Jinqi; Sun, Jiashu*

Acta Chim. Sinica **2022**, *80*(5), 679-689

Different thermomicrofluidic biosensing strategies, including microscale thermophoresis (MST), thermophoresis-convection coupling, thermophoresis-diffusiophoresis coupling and thermophoresis-electrophoresis coupling, were presented. The fundamentals, features, and applications of these strategies in detecting biomolecules (protein, nucleic acids, *etc.*) and biological micro/nanoparticles (extracellular vesicles, viral particles, cells, *etc.*) were summarized. The challenge and future directions for the application of thermomicrofluidic biosensing in biomedical detection were discussed.

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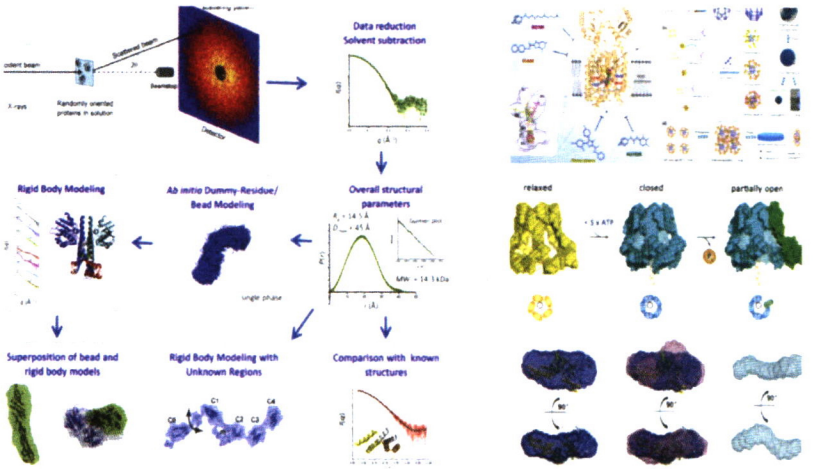
Solution Small-Angle Scattering in Soft Matter: Application and Prospective



Solution small-angle scattering (SAS) is a powerful tool for elucidating the structural properties of soft matter systems. In recent years, solution SAS techniques have had versatile applications in several research fields, especially in structural biology and in probing self-assembling nanomaterials. Probing the structure of materials at micro- and nano-scales provide an insight on the macroscopic properties of the material. The high throughput and fast time resolution offered by SAS includes X-ray scattering (SAXS) in combination with the neutron penetrating ability in Neutron scattering (SANS) can offer a great potential to cover different soft-matter systems and processes (*i.e.* probing the kinetic of self-assembly). Given the potential offered by the next generation X-ray and Neutron sources, further developments in this field are expected, with a proliferation of solution SAS applications.

Song, Panqi; Zhang, Jianqiao; Li, Yiwen; Liu, Guangfeng; Li, Na*

Acta Chim. Sinica **2022**, *80*(5), 690-702

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ISSN 0567-7351
CN 31-1320/O6
CODEN HHHPA4
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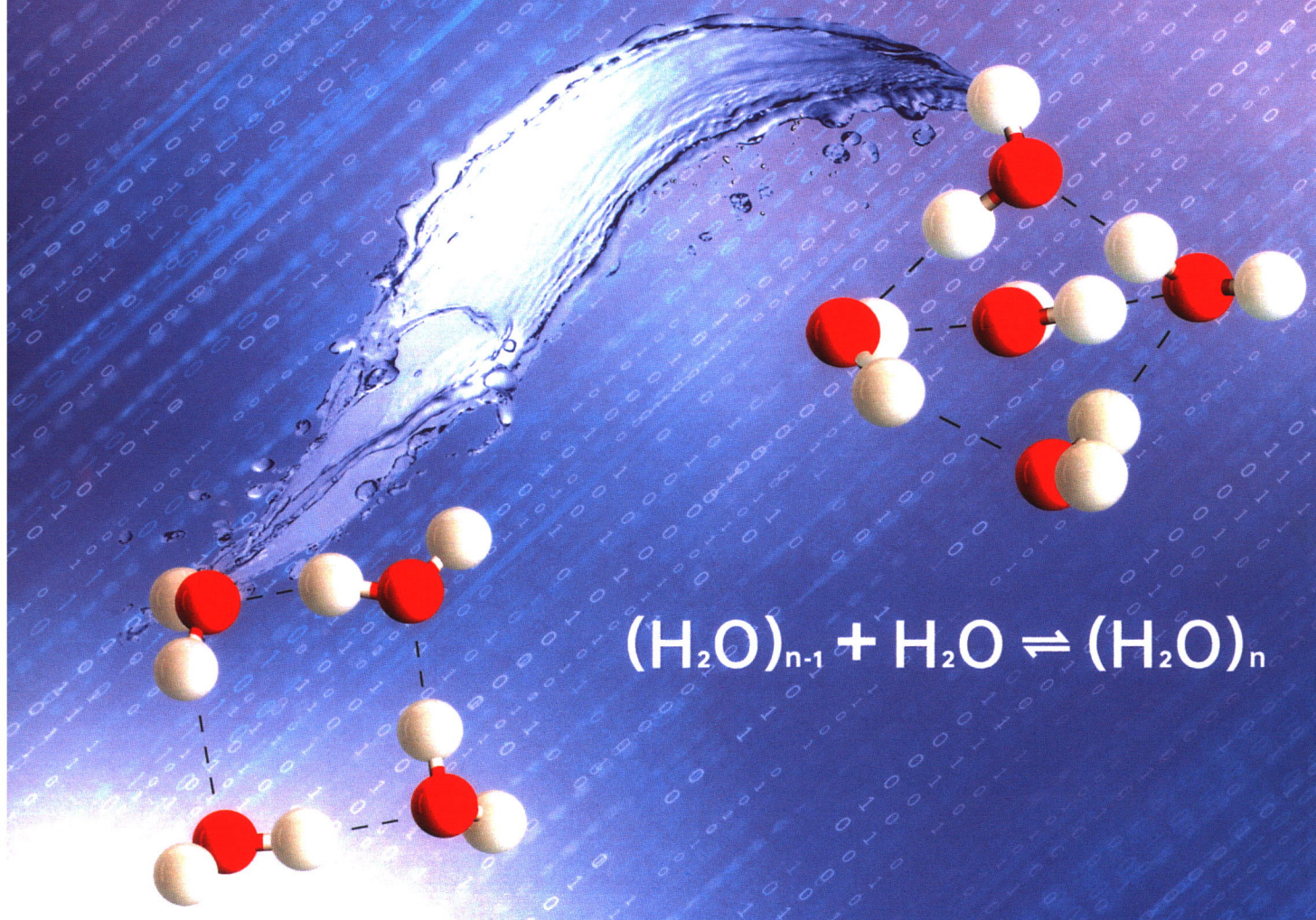
ACTA CHIMICA SINICA

Volume 80 Number 5 May 2022



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万方数据

国际刊号：ISSN 0567-7351 国内刊号：CN 31-1320/O6 国内邮发代号：4-209 国外发行代号：M56