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物理化学学报

ACTA PHYSICO-CHIMICA SINICA

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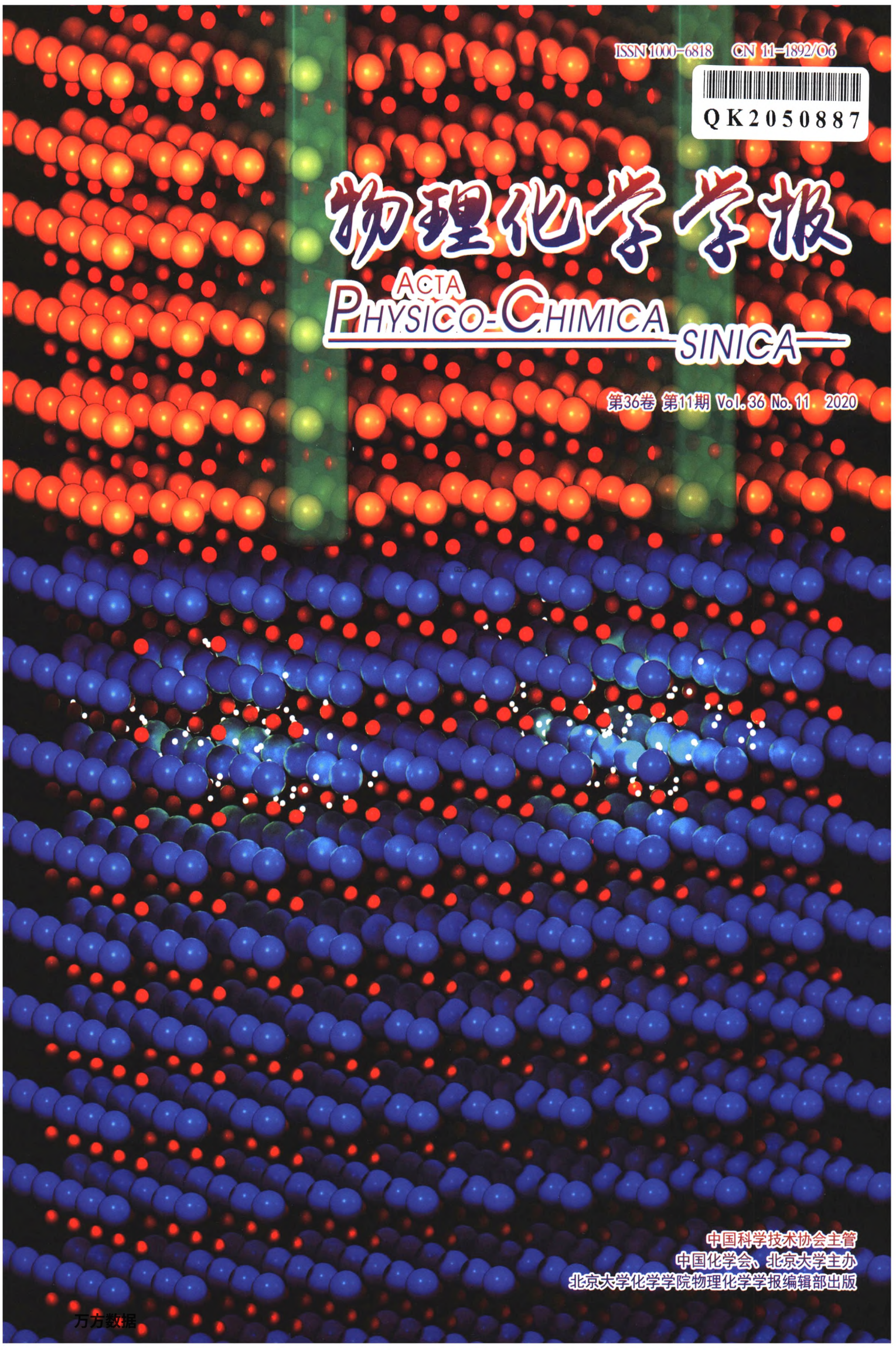

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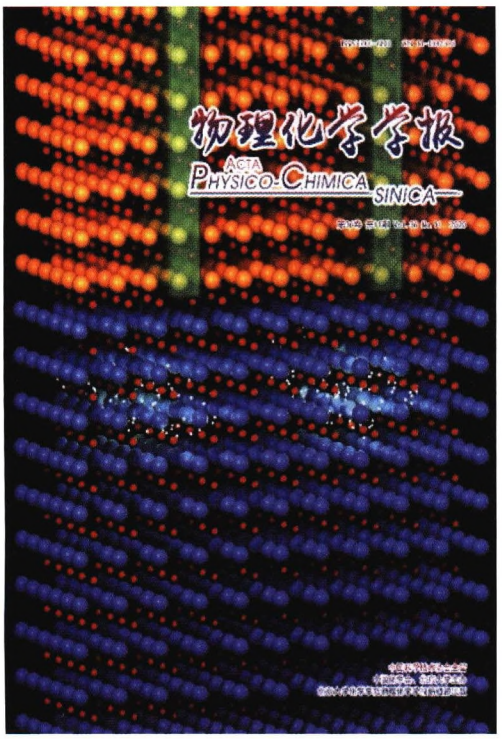
物 理 化 学 学 报 第 36 卷 第 11 期
ACTA PHYSICO-CHIMICA SINICA, Vol. 36, No. 11

COVER



The cover image shows the application of aberration-corrected scanning transmission electron microscope (STEM) and electron energy-loss spectroscopy (EELS) in exploring the atomic and electronic structure of heterointerface. In article No. 1906019, Tian *et al.* demonstrate that the aggregation of electron near the a[001] cores of the periodic misfit dislocation will probably increase the electron conductivity along the dislocation line.

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亮点 HIGHLIGHT

当期推荐　RECOMMENDATION

综述　REVIEW

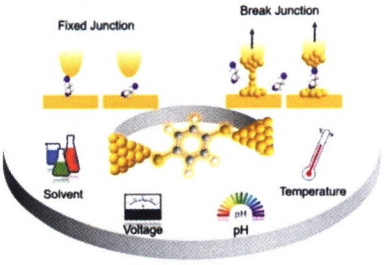
单分子电导测量技术及其影响因素

程鹏坤，李云川，常帅

Techniques and Influencing Factors for Single Molecule Electronic Conductance Measurements

Pengkun Cheng, Yunchuan Li, Shuai Chang

Acta Phys. -Chim. Sin. **2020,** *36* (11), 1909043
doi: 10.3866/PKU.WHXB201909043



Techniques and influencing factors for single molecule electronic conductance measurements are systematically summarized.

论文　ARTICLE

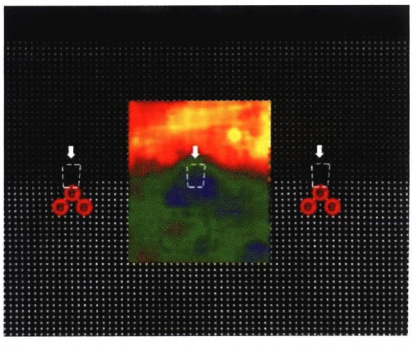
PbTiO$_3$/SrTiO$_3$(010)异质界面上的周期性失配位错及电子富集

陈星，田鹤，张泽

Periodic Misfit Dislocation and Electron Aggregation at (010) PbTiO$_3$/SrTiO$_3$ Heterointerface

Xing Chen, He Tian, Ze Zhang

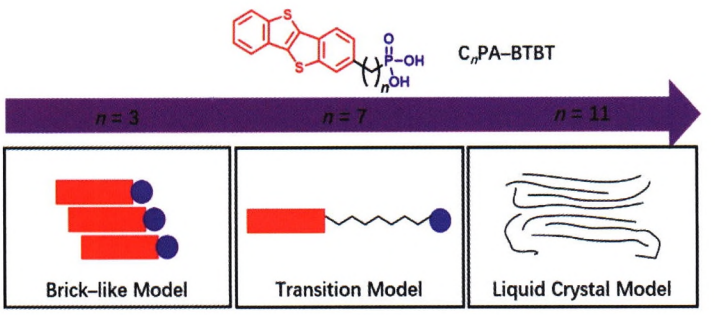
Acta Phys. -Chim. Sin. **2020,** *36* (11), 1906019
doi: 10.3866/PKU.WHXB201906019



The possible aggregation of electrons near the *a*[001] dislocation cores at (010) PbTiO$_3$/SrTiO$_3$ heterointerface was found using STEM and EELS.

烷基链工程对两亲有机半导体热力学性能影响的研究

李明亮，李硕，王国治，郭雪峰



Effects of Alkyl-Chain Engineering on the Thermodynamic Properties of Amphiphilic Organic Semiconductors

Mingliang Li, Shuo Li, Guozhi Wang, Xuefeng Guo

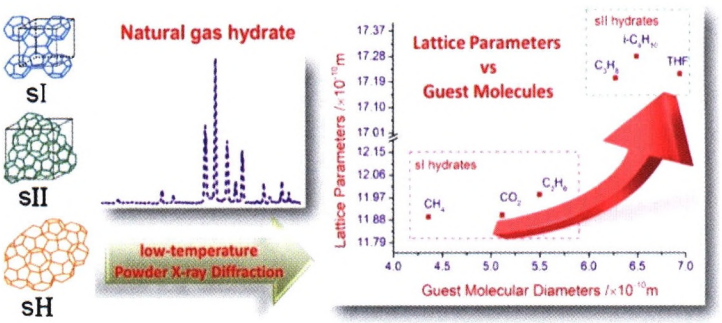
Acta Phys. -Chim. Sin. **2020,** *36* (11), 1908036

doi: 10.3866/PKU.WHXB201908036

Based on alkyl-chain engineering, a series of amphiphilic functional molecules were proposed. A molecular model was established according to the thermodynamic study based on TGA and DSC.

常见客体分子对笼型水合物晶格常数的影响

孟庆国，刘昌岭，李承峰，郝锡荦，胡高伟，孙建业，吴能友



Effect of Common Guest Molecules on the Lattice Constants of Clathrate Hydrates

Qingguo Meng, Changling Liu, Chengfeng Li, Xiluo Hao, Gaowei Hu, Jianye Sun, Nengyou Wu

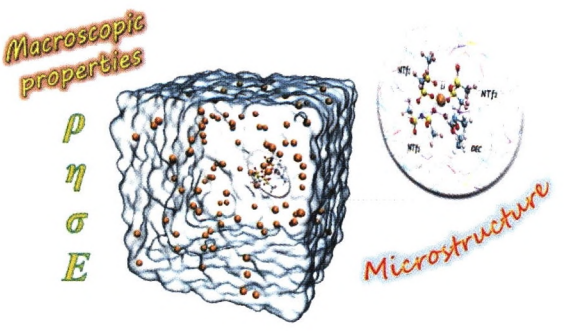
Acta Phys. -Chim. Sin. **2020,** *36* (11), 1910010

doi: 10.3866/PKU.WHXB201910010

The influences of different guest molecules on the lattice constants of clathrate hydrates are determined by low-temperature powder X-ray diffraction analysis.

[C$_3$mim][NTf$_2$]/DEC/[Li][NTf$_2$]体系的基础性质

惠淑荣，赵丽薇，刘青山，宋大勇



Basic Properties of [C$_3$mim][NTf$_2$]/DEC/[Li][NTf$_2$] Systems

Shurong Hui, Liwei Zhao, Qingshan Liu, Dayong Song

Acta Phys. -Chim. Sin. **2020,** *36* (11), 1910067

doi: 10.3866/PKU.WHXB201910067

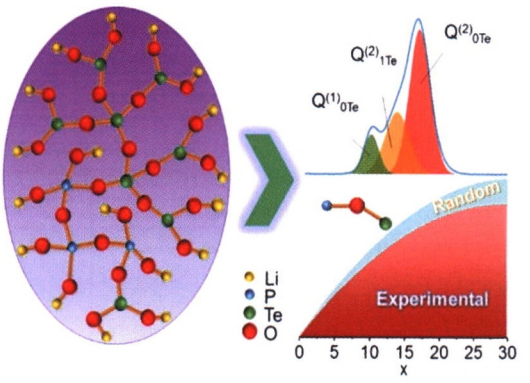
The interaction between $[Li]^+$ and $[NTf_2]^-$ is weakened with increasing DEC content in the system.

利用固态核磁共振研究 $100LiO_{1/2}$-$(100-x)PO_{5/2}$-$xTeO_2$ 快离子导电玻璃的结构

张宗辉，任进军，胡丽丽

Structure Investigations on $100LiO_{1/2}$-$(100-x)PO_{5/2}$-$xTeO_2$ Fast Ionic Conducting Glasses Using Solid-State Nuclear Magnetic Resonance Spectroscopy

Zonghui Zhang, Jinjun Ren, Lili Hu



Acta Phys. -Chim. Sin. **2020,** *36* (11), 2001048

doi: 10.3866/PKU.WHXB202001048

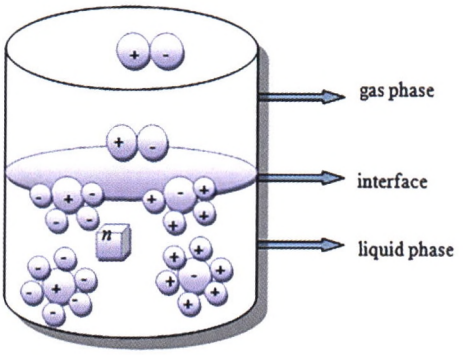
The glass structures were probed using SSNMR, and the connectivities of glass networks were analyzed using a random distribution model.

1-烷基-3-甲基咪唑氯化物焓变的热重分析

刘璐，徐玉萍，陈霞，洪梅，佟静

Thermogravimetric Analysis of Enthalpy Variation of 1-Alkyl-3-methylimidazole Chloride

Lu Liu, Yuping Xu, Xia Chen, Mei Hong, Jing Tong



Acta Phys. -Chim. Sin. **2020,** *36* (11), 2004014

doi: 10.3866/PKU.WHXB202004014

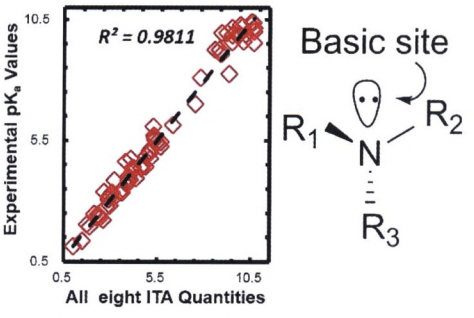
Changing the anion will affect vaporization enthalpy of ionic liquids due to the existence of intermolecular hydrogen bonds.

运用概念密度泛函理论和信息论方法定量描述胺类分子的分子碱度

肖雪珠，曹小芳，赵东波，荣春英，刘述斌

Quantification of Molecular Basicity for Amines: a Combined Conceptual Density Functional Theory and Information-Theoretic Approach Study

Xuezhu Xiao, Xiaofang Cao, Dongbo Zhao, Chunying Rong, Shubin Liu



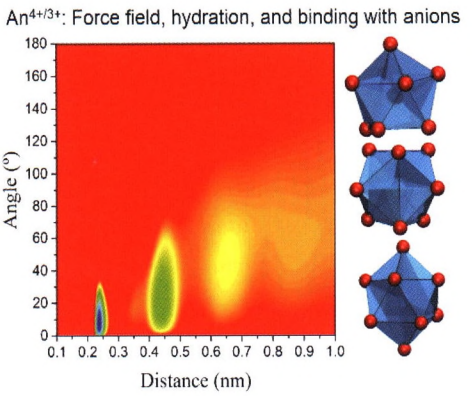
Acta Phys. -Chim. Sin. **2020,** *36* (11), 1906034

doi: 10.3866/PKU.WHXB201906034

Quantities from conceptual density functional theory and information-theoretic approach can predict molecular basicity of primary, secondary, and tertiary amines, as demonstrated from our study on 179 molecular systems.

镎(IV)、镅(III)、锔(III)的 AMBER 力场参数化及评估

刘子义，夏苗仁，柴之芳，王东琪



Parameterization and Validation of AMBER Force Field for Np^{4+}, Am^{3+}, and Cm^{3+}

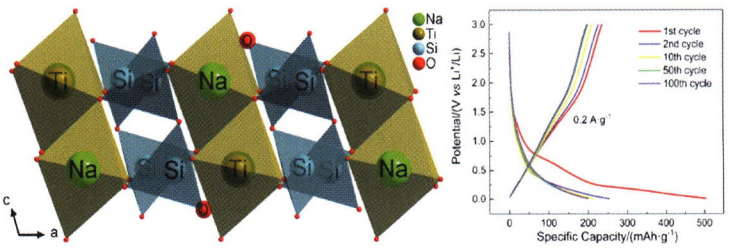
Ziyi Liu, Miaoren Xia, Zhifang Chai, Dongqi Wang

Acta Phys. -Chim. Sin. **2020,** *36* (11), 1908035
doi: 10.3866/PKU.WHXB201908035

The AMBER force field of Np^{4+}, Am^{3+}, and Cm^{3+} was parameterized and applied to investigate their hydration and coordination behavior with typical inorganic anions.

$NaTiSi_2O_6$/C 复合材料用于锂离子电池负极材料

刘昆，刘瑶，朱海峰，董晓丽，王永刚，王丛笑，夏永姚



$NaTiSi_2O_6$/C Composite as a Novel Anode Material for Lithium-Ion Batteries

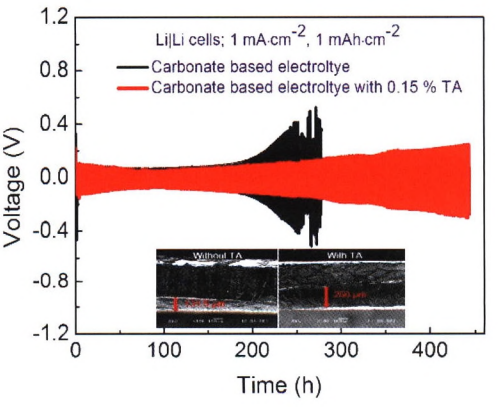
Kun Liu, Yao Liu, Haifeng Zhu, Xiaoli Dong, Yonggang Wang, Congxiao Wang, Yongyao Xia

Acta Phys. -Chim. Sin. **2020,** *36* (11), 1912030
doi: 10.3866/PKU.WHXB201912030

A novel silicate anode material $NaTiSi_2O_6$ was successfully synthesized and tested in lithium-ion batteries.

多酚类化合物—丹宁酸用作锂金属负极电解液成膜添加剂

冉琴，孙天霭，韩冲宇，张浩楠，颜剑，汪靖伦



Natural Polyphenol Tannic Acid as an Efficient Electrolyte Additive for High Performance Lithium Metal Anode

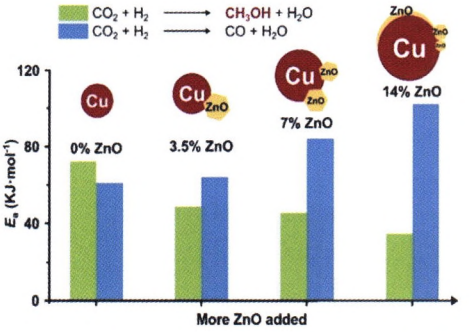
Qin Ran, Tianyang Sun, Chongyu Han, Haonan Zhang, Jian Yan, Jinglun Wang

Acta Phys. -Chim. Sin. **2020,** *36* (11), 1912068
doi: 10.3866/PKU.WHXB201912068

A planar micro-battery was designed to study the lithiation behaviors of few-layered graphene sheets by Raman mapping.

ZnO 逆修饰小尺寸 Cu/SiO_2 催化剂及其在 CO_2 加氢制甲醇中的应用

吕翰林，胡兵，刘国亮，洪昕林，庄林



Inverse Decoration of ZnO on Small-Sized Cu/Sio_2 with Controllable Cu-ZnO Interaction for CO_2 Hydrogenation to Produce Methanol

Hanlin Lyu, Bing Hu, Guoliang Liu, Xinlin Hong, Lin Zhuang

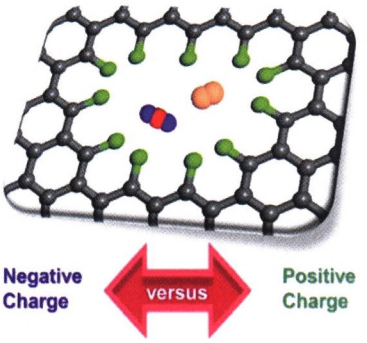
Acta Phys. -Chim. Sin. **2020,** *36* (11), 1911008

doi: 10.3866/PKU.WHXB201911008

This work shows the potential application of copper silicate to fabricate Cu-ZnO catalysts and confirms the remarkable influence of ZnO on the Cu particle size, which further affects the activity of the catalyst for CO_2 reduction toward methanol production.

基于静电效应的石墨烯纳米孔选择性渗透特性

孙成珍，周润峰，白博峰



Electrostatic Effect-based Selective Permeation Characteristics of Graphene Nanopores

Chengzhen Sun, Runfeng Zhou, Bofeng Bai

Acta Phys. -Chim. Sin. **2020,** *36* (11), 1911044

doi: 10.3866/PKU.WHXB201911044

Negative surface charges can induce the electrostatic effect-based CO_2/N_2 selectivity through graphene nanopores, while the positive charges cannot induce it.

评论　EDITORIAL

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