

JANUARY 15, 2015

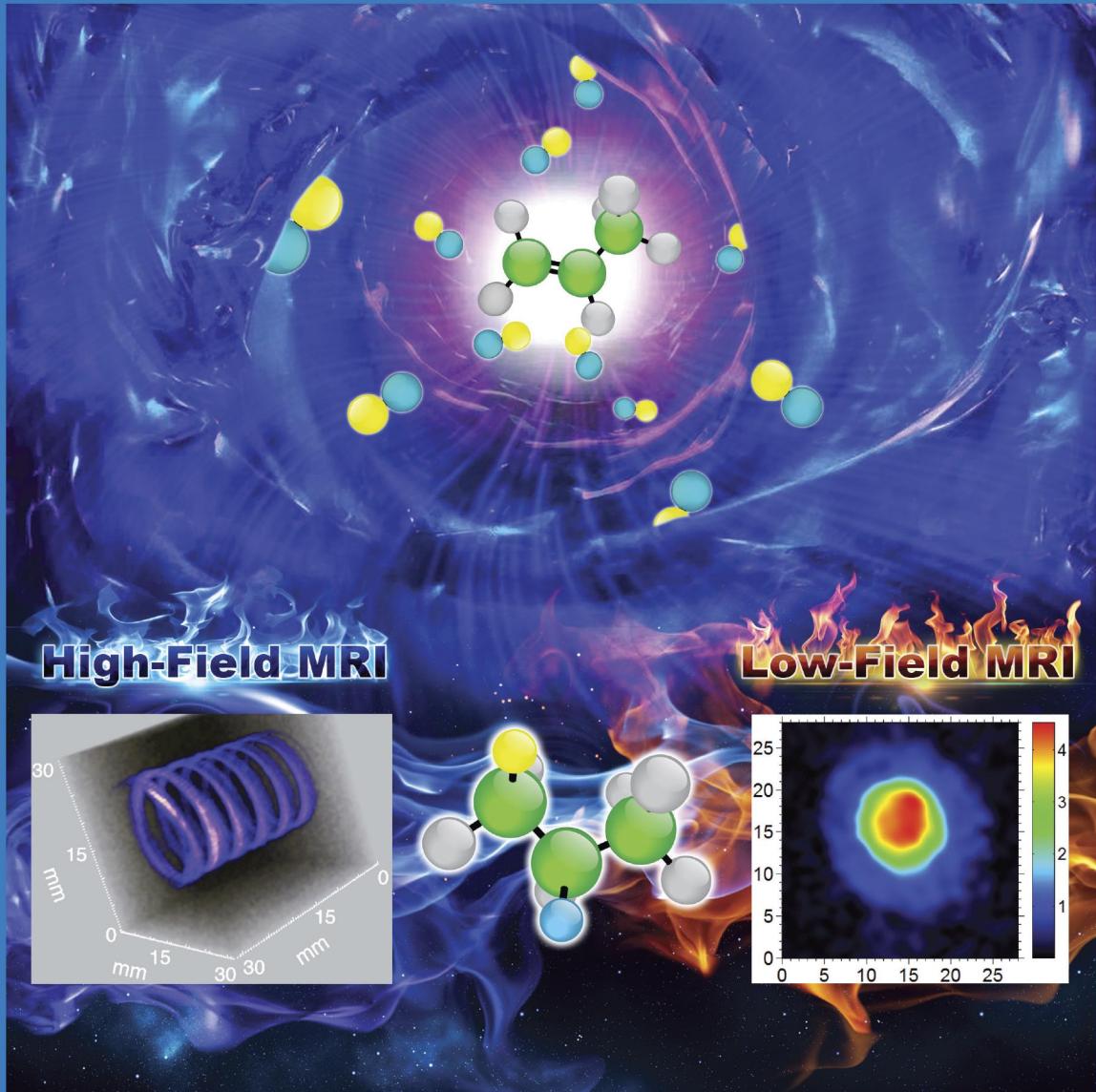
VOLUME 119

NUMBER 2

pubs.acs.org/JPCCTHE JOURNAL OF
PHYSICAL
CHEMISTRY

C

Parahydrogen-Induced
Polarization of
Propane- d_6 Gas for
Biomedical Imaging
Applications and Beyond
(see page 5A)



ENERGY CONVERSION AND STORAGE, OPTICAL AND ELECTRONIC DEVICES,
INTERFACES, NANOMATERIALS, AND HARD MATTER



ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org

THE JOURNAL OF PHYSICAL CHEMISTRY C

January 15, 2015: Vol. 119, Iss. 2

Content

- Oxygen Plasma Induced Hierarchically Structured Gold Electrocatalyst for Selective Reduction of Carbon Dioxide to Carbon Monoxide**

Jai Hyun Koh, Hyo Sang Jeon, Michael Shincheon Jee, Eduardus Budi Nursanto, Hyunjoo Lee, Yun Jeong Hwang, and Byoung Koun Min

The Journal of Physical Chemistry C 2015 119 (2), 883-889

- Electron Transfer to Light-Activated Photosynthetic Reaction Centers from Rhodobacter sphaeroides Reconstituted in a Biomimetic Membrane System**

Jens Gebert, Ciril Reiner-Rozman, Christoph Steininger, Vedran Nedelkovski, Christoph Nowak, Colin A. Wright, and Renate L. C. Naumann

The Journal of Physical Chemistry C 2015 119 (2), 890-895

- Understanding Lithium Inventory Loss and Sudden Performance Fade in Cylindrical Cells during Cycling with Deep-Discharge Steps**

E. Sarasketa-Zabala, F. Aguesse, I. Villarreal, L. M. Rodriguez-Martinez, C. M. López, and P. Kubiak

The Journal of Physical Chemistry C 2015 119 (2), 896-906

- Origins for the Synergetic Effects of AuCu3 in Catalysis for Oxygen Reduction Reaction**

Nanlin Zhang, Huijun Yan, Xin Chen, Li An, Zhonghong Xia, and Dingguo Xia

The Journal of Physical Chemistry C 2015 119 (2), 907-912

- Improvement on Hydrogen Desorption Performance of Calcium Borohydride Diammoniate Doped with Transition Metal Chlorides**

Hailiang Chu, Shujun Qiu, Yongjin Zou, Cuili Xiang, Huanzhi Zhang, Fen Xu, Lixian Sun, and Huaiying Zhou

The Journal of Physical Chemistry C 2015 119 (2), 913-918

- Insight into Lithium Diffusion in Conversion-Type Iron Oxide Negative Electrode**

Bingbing Tian, Jolanta Świątowska, Vincent Maurice, Catarina Pereira-Nabais, Antoine Seyeux, and Philippe Marcus

The Journal of Physical Chemistry C 2015 119 (2), 919-925

7. Cooperativity in a New Role: Stabilization of the Ammonium Salts in the Solid State over Their H-Bonded Complexes in the Gas Phase

Saied Md. Pratik, Sourav Chakraborty, Sourav Mandal, and Ayan Datta
The Journal of Physical Chemistry C 2015 119 (2), 926-933

8. First Direct Study of the Ammonolysis Reaction in the Most Common Alkaline and Alkaline Earth Metal Hydrides by in Situ SR-PXD

C. Pistidda, A. Santoru, S. Garroni, N. Bergemann, A. Rzeszutek, C. Horstmann, D. Thomas, T. Klassen, and M. Dornheim
The Journal of Physical Chemistry C 2015 119 (2), 934-943

9. Observation and Investigation of Increasing Isosteric Heat of Adsorption of Ethane on Zeolite-Templated Carbon

Maxwell Murialdo, Nicholas P. Stadie, Channing C. Ahn, and Brent Fultz
The Journal of Physical Chemistry C 2015 119 (2), 944-950

10. Oxidative Tearing of Graphene Sheets: Insights into the Probable Situations by Computational and Experimental Studies

Angana Ray, Kousik Bagani, Sangam Banerjee, and Dhananjay Bhattacharyya
The Journal of Physical Chemistry C 2015 119 (2), 951-959

11. Defect Scaling with Contact Area in EGaIn-Based Junctions: Impact on Quality, Joule Heating, and Apparent Injection Current

Li Jiang, C. S. Suchand Sangeeth, Albert Wan, Ayelet Vilan, and Christian A. Nijhuis
The Journal of Physical Chemistry C 2015 119 (2), 960-969

12. Physical Properties of a New Deep Eutectic Solvent Based on a Sulfonium Ionic Liquid as a Suitable Electrolyte for Electric Double-Layer Capacitors

Xiong Baokou and Mériem Anouti
The Journal of Physical Chemistry C 2015 119 (2), 970-979

13. Electron-Acceptor-Dependent Light Absorption and Charge-Transfer Dynamics in N-Annulated Perylene Dye-Sensitized Solar Cells

Lin Yang, Yameng Ren, Zhaoyang Yao, Cancan Yan, Wentao Ma, and Peng Wang
The Journal of Physical Chemistry C 2015 119 (2), 980-988

14. Transient Bimodal Particle Size Distributions during Pt Sintering on Alumina and Silica

Pooya Tabib Zadeh Adibi, Vladimir P. Zhdanov, Christoph Langhammer, and Henrik Grönbeck
The Journal of Physical Chemistry C 2015 119 (2), 989-996

15.Thermodynamic Model of Charging the Gas/Water Interface

Nikola Kallay, Tajana Preočanin, Atiđa Selmani, Davor Kovačević, Johannes Lützenkirchen, Hiromichi Nakahara, and Osamu Shibata
The Journal of Physical Chemistry C 2015 119 (2), 997-1007

16.Comparative Study of Acidic Properties of UZM-5 Nanosheets by Stepwise Adsorption Assisted by a Selective External Poisoning Approach

Sen Lin, Lei Shi, and Tingting Yu
The Journal of Physical Chemistry C 2015 119 (2), 1008-1015

17.Dehydrogenation of Propane to Propylene by a Pd/Cu Single-Atom Catalyst: Insight from First-Principles Calculations

Xinrui Cao, Yongfei Ji, and Yi Luo
The Journal of Physical Chemistry C 2015 119 (2), 1016-1023

18.Li₂O₂ Wetting on the (110) Surface of RuO₂, TiO₂, and SnO₂: An Initiating Force for Polycrystalline Growth

W. T. Geng and T. Ohno
The Journal of Physical Chemistry C 2015 119 (2), 1024-1031

19.Influence of Adsorbed Water on the Oxygen Evolution Reaction on Oxides

S. Siahrostami and A. Vojvodic
The Journal of Physical Chemistry C 2015 119 (2), 1032-1037

20.Self-Assembly of Peptide Nanostructures onto an Electrode Surface for Nonenzymatic Oxygen Sensing

Camila P. Sousa, Mauricio D. Coutinho-Neto, Michelle S. Liberato, Lauro T. Kubota, and Wendel A. Alves
The Journal of Physical Chemistry C 2015 119 (2), 1038-1046

21.Understanding the Stabilization of Single-Walled Carbon Nanotubes and Graphene in Ionic Surfactant Aqueous Solutions: Large-Scale Coarse-Grained Molecular Dynamics Simulation-Assisted DLVO Theory

Chih-Jen Shih, Shangchao Lin, Michael S. Strano, and Daniel Blankschtein
The Journal of Physical Chemistry C 2015 119 (2), 1047-1060

22.Photo-Induced Doping in Graphene/Silicon Heterostructures

Xiao-Juan Wang, Liping Zou, Dong Li, Qichong Zhang, Fengli Wang, and Zengxing Zhang
The Journal of Physical Chemistry C 2015 119 (2), 1061-1066

23. Temperature-Dependent Transport Properties of a Redox-Active Ionic Liquid with a Viologen Group

Nataraju Bodappa, Peter Broekmann, Yong-Chun Fu, Julien Furrer, Yutaro Furue, Takamasa Sagara, Hans Siegenthaler, Hironobu Tahara, Soma Vesztergom, Klaus Zick, and Thomas Wandlowski

The Journal of Physical Chemistry C 2015 119 (2), 1067-1077

24. Understanding the H₂ Sorption Trends in the M-MOF-74 Series (M = Mg, Ni, Co, Zn)

Tony Pham, Katherine A. Forrest, Rahul Banerjee, Gisela Orcajo, Juergen Eckert, and Brian Space

The Journal of Physical Chemistry C 2015 119 (2), 1078-1090

25. Room Temperature Atomic Layer-like Deposition of ZnO on Functionalized Self-Assembled Monolayers

Zhiwei Shi and Amy V. Walker

The Journal of Physical Chemistry C 2015 119 (2), 1091-1100

26. Shape-Dependence of Pd Nanocrystal Carburization during Acetylene Hydrogenation

Micaela Crespo-Quesada, Songhak Yoon, Mingshang Jin, Antonio Prestianni, Remedios Cortese, Fernando Cárdenas-Lizana, Dario Duca, Anke Weidenkaff, and Lioubov Kiwi-Minsker
The Journal of Physical Chemistry C 2015 119 (2), 1101-1107

27. Incommensurate Growth of Thin and Ultrathin Films of Single-Phase Fe₃O₄(001) on SrTiO₃(001)

Juan Rubio-Zuazo, Laura Onandia, Eduardo Salas-Colera, Alvaro Muñoz-Noval, and German R. Castro

The Journal of Physical Chemistry C 2015 119 (2), 1108-1112

28. Reactions of Deuterated Methanol (CD₃OD) on Fe₃O₄(111)

Zhisheng Li, Denis V. Potapenko, Kwang Taeg Rim, Maria Flytzani-Stephanopoulos, George W. Flynn, Richard M. Osgood, Xiao-Dong Wen, and Enrique R. Batista

The Journal of Physical Chemistry C 2015 119 (2), 1113-1120

29. Hydrogen Adsorption on Small Zeolite-Supported Rhodium Clusters. A Density Functional Study

Velina K. Markova, Georgi N. Vayssilov, and Notker Rösch

The Journal of Physical Chemistry C 2015 119 (2), 1121-1129

30. Ammonia Formation from NO Reaction with Surface Hydroxyls on Rutile TiO₂(110)-1 × 1

Boseong Kim, Bruce D. Kay, Zdenek Dohnálek, and Yu Kwon Kim

The Journal of Physical Chemistry C 2015 119 (2), 1130-1135

31. Density Functional Studies of Stoichiometric Surfaces of Orthorhombic Hybrid Perovskite CH₃NH₃PbI₃

Yun Wang, Bobby G. Sumpter, Jingsong Huang, Haimin Zhang, Porun Liu, Huagui Yang, and Huijun Zhao

The Journal of Physical Chemistry C 2015 119 (2), 1136-1145

32. Dual Mechanism of Indium Incorporation into TiO₂ (Rutile)

Janusz Nowotny, Tadeusz Bak, and Mohammad A. Alim

The Journal of Physical Chemistry C 2015 119 (2), 1146-1154

33. Sulfated Temperature Effects on the Catalytic Activity of CeO₂ in NH₃-Selective Catalytic Reduction Conditions

Lei Zhang, Weixin Zou, Kaili Ma, Yuan Cao, Yan Xiong, Shiguo Wu, Changjin Tang, Fei Gao, and Lin Dong

The Journal of Physical Chemistry C 2015 119 (2), 1155-1163

34. Is Ice Nucleation from Supercooled Water Insensitive to Surface Roughness?

James M. Campbell, Fiona C. Meldrum, and Hugo K. Christenson

The Journal of Physical Chemistry C 2015 119 (2), 1164-1169

35. Recombination of Formaldehyde and Hydrogen Atoms on TiO₂(110)

Xinchun Mao, Dong Wei, Zhiqiang Wang, Xianchi Jin, Qunqing Hao, Zefeng Ren, Dongxu Dai, Zhibo Ma, Chuanyao Zhou, and Xueming Yang

The Journal of Physical Chemistry C 2015 119 (2), 1170-1174

36. Upconversion Luminescence of Rare-Earth-Doped Y₂O₃ Nanoparticle with Metal Nano-Cap

Kaoru Yamamoto, Minoru Fujii, Shunji Sowa, Kenji Imakita, and Kanna Aoki

The Journal of Physical Chemistry C 2015 119 (2), 1175-1179

37. Tunable Surface Plasmon Resonance in Sn-Doped Zn–Cd–O Alloyed Nanocrystals

Sirshendu Ghosh, Manas Saha, Vishal Dev Ashok, Biswajit Dalal, and S. K. De

The Journal of Physical Chemistry C 2015 119 (2), 1180-1187

38. Theoretical Study on the Enhancement of the Second Hyperpolarizabilities of Si-, Ge-Disubstituted Quinodimethanes: Synergy Effects of Open-Shell Nature and Intramolecular Charge Transfer

Kotaro Fukuda, Takeshi Nozawa, Hiroko Yotsuyanagi, Masaaki Ichinohe, Akira Sekiguchi, and Masayoshi Nakano

The Journal of Physical Chemistry C 2015 119 (2), 1188-1193

39. Size Dependence of Crystal Structure and Magnetic Properties of NiO Nanoparticles in Mesoporous Silica

Takayuki Tajiri, Seiya Saisho, Masaki Mito, Hiroyuki Deguchi, Kensuke Konishi, and Atsushi Kohno
The Journal of Physical Chemistry C 2015 119 (2), 1194-1200

40. Morphology of Supported Polymer Electrolyte Ultrathin Films: A Numerical Study

Daiane Damasceno Borges, Gerard Gebel, Alejandro A. Franco, Kourosh Malek, and Stefano Mossa
The Journal of Physical Chemistry C 2015 119 (2), 1201-1216

41. Role of Au₄ Units on the Electronic and Bonding Properties of Au₂₈(SR)₂₀ Nanoclusters from X-ray Spectroscopy

Daniel M. Chevrier, Chenjie Zeng, Rongchao Jin, Amares Chatt, and Peng Zhang
The Journal of Physical Chemistry C 2015 119 (2), 1217-1223

42. Spin Dynamics in Hybrid Iron Oxide–Gold Nanostructures

Tomas Orlando, A. Capozzi, E. Umut, L. Bordonali, M. Mariani, P. Galinetto, F. Pineider, C. Innocenti, P. Masala, F. Tabak, M. Scavini, P. Santini, M. Corti, C. Sangregorio, P. Ghigna, and A. Lascialfari
The Journal of Physical Chemistry C 2015 119 (2), 1224-1233

43. Fabrication of Si/Au Core/Shell Nanoplasmonic Structures with Ultrasensitive Surface-Enhanced Raman Scattering for Monolayer Molecule Detection

Pu Liu, Huanjun Chen, Hao Wang, Jiahao Yan, Zhaoyong Lin, and Guowei Yang
The Journal of Physical Chemistry C 2015 119 (2), 1234-1246

44. Interlayer Electronic Coupling in Arbitrarily Stacked MoS₂ Bilayers Controlled by Interlayer S–S Interaction

Boxiao Cao and Tianshu Li
The Journal of Physical Chemistry C 2015 119 (2), 1247-1252

45. Composition-Dependent Light-Induced Dipole Moment Change in Organometal Halide Perovskites

Xiaojing Wu, Hui Yu, Linkai Li, Feng Wang, Haihua Xu, and Ni Zhao
The Journal of Physical Chemistry C 2015 119 (2), 1253-1259

46. One- and Two-Photon Absorption in CdS Nanodots and Wires: The Role of Dimensionality in the One- and Two-Photon Luminescence Excitation Spectrum

Alexander W. Achtstein, Ana Ballester, Jose L. Movilla, Jonas Hennig, Juan I. Climente, Anatol Prudnikau, Artsiom Antanovich, Riccardo Scott, Mikhail V. Artemyev, Josep Planelles, and Ulrike

Woggon
The Journal of Physical Chemistry C 2015 119 (2), 1260-1267

47. Correction to “Formation and Characterization of Femtosecond-Laser-Induced Subcluster Segregated Nanoalloys”

Zhen Jiao, Mugunthan Sivayoganathan, Walter W. Duley, Peng He, and Y. Norman Zhou
The Journal of Physical Chemistry C 2015 119 (2), 1268-1268

48. Corrections to Surface Reconstruction and Reactivity of Platinum-Iron Oxide Nanoparticles

Paul N. Duchesne, Guangxu Chen, Xiaojing Zhao, Nanfeng Zheng, and Peng Zhang
The Journal of Physical Chemistry C 2015 119 (2), 1269-1269

49. Correction to “Growth of 2D ZnO Nanowall for Energy Harvesting Application”

Balasubramaniam Saravanakumar and Sang-Jae Kim
The Journal of Physical Chemistry C 2015 119 (2), 1270-1270