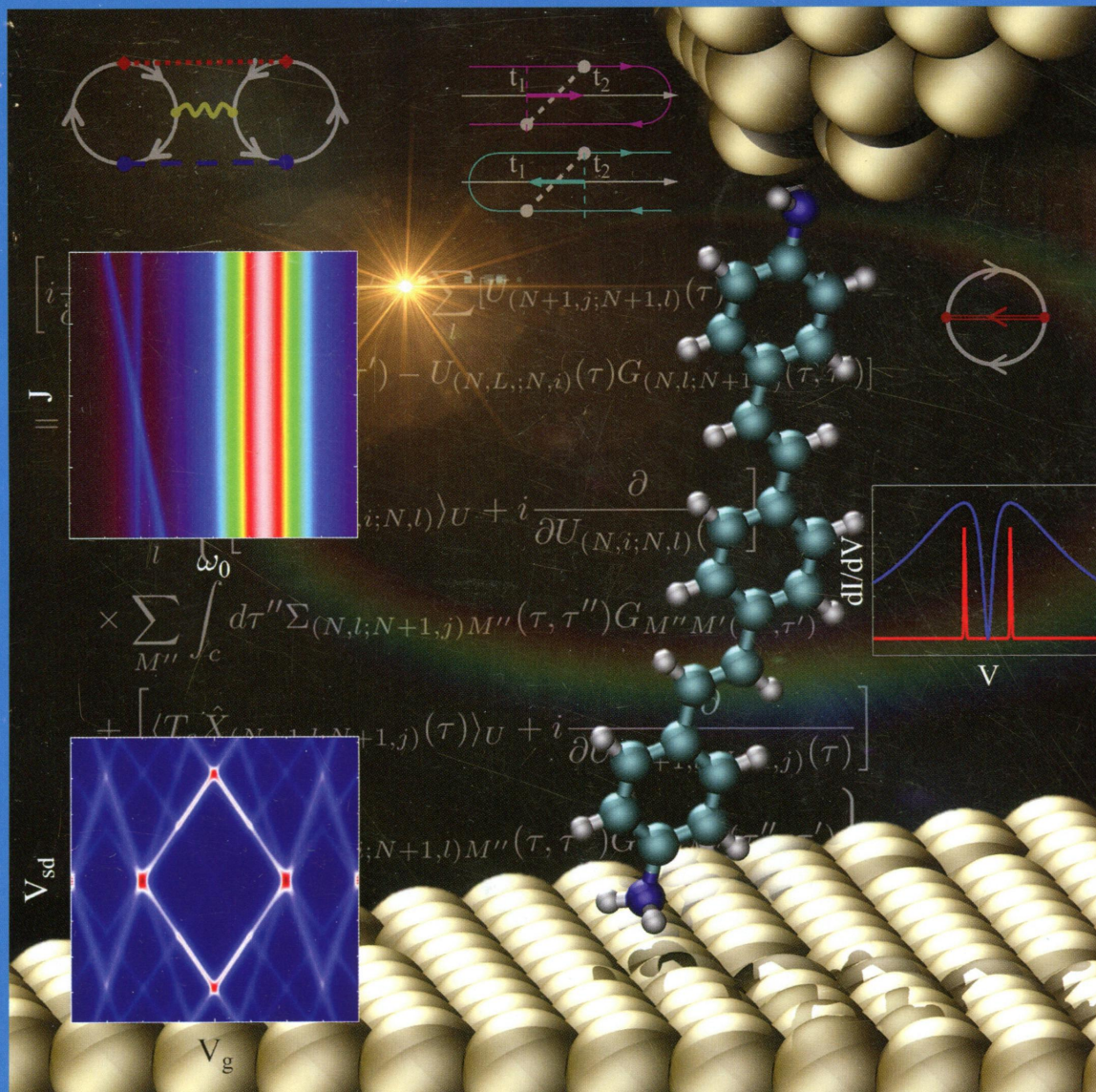


THE JOURNAL OF PHYSICAL CHEMISTRY

C

Molecular Many-Body States Formulation, the Nonequilibrium Atomic Limit, for Transport and Optical Response in Molecular Junctions (see page 11159)



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



ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org

ON THE COVER: Molecular many-body states formulation, the nonequilibrium atomic limit, for transport and optical response in molecular junctions. Theoretical formulations of nonequilibrium open systems usually rely on language of elementary excitations (quasiparticles). An alternative approach, the nonequilibrium atomic limit, utilizes many-body states of the system. Such approach is especially convenient in theoretical description of response in molecular junctions, where methods of the quantum chemistry are combined with the quantum transport theory. See page 11159.

Feature Article

11159

[dx.doi.org/10.1021/jp500880j](https://doi.org/10.1021/jp500880j)

Nonequilibrium Atomic Limit for Transport and Optical Response of Molecular Junctions

Alexander J. White, Maicol A. Ochoa, and Michael Galperin*

Articles

Energy Conversion and Storage; Energy and Charge Transport

11174

[dx.doi.org/10.1021/jp4110536](https://doi.org/10.1021/jp4110536)

Niobium Segregation in Niobium-Doped Titanium Dioxide (Rutile)

Armand J. Atanacio, Tadeusz Bak, and Janusz Nowotny*

11186

[dx.doi.org/10.1021/jp412699w](https://doi.org/10.1021/jp412699w)

Optical and Acoustic Phonon Dynamics of Exciton Self-Trapping in a Nondegenerate Quasi-One-Dimensional Charge Density Wave System

J. G. Mance, J. J. Felver, and S. L. Dexheimer*

11193

[dx.doi.org/10.1021/jp500318e](https://doi.org/10.1021/jp500318e)

Crystal Structures, Phase Stability, and Decomposition Reactions in the Quaternary Mg–B–N–H Hydrogen Storage System

Yongsheng Zhang,* David Farrell, Jun Yang, Andrea Sudik, and C. Wolverton

11203


[dx.doi.org/10.1021/jp5004402](https://doi.org/10.1021/jp5004402)

Initial Assessment of an Empirical Potential as a Portable Tool for Rapid Investigation of Li⁺ Diffusion in Li⁺-Battery Cathode Materials

Ramzi Kutteh* and Maxim Avdeev

- 11215 [dx.doi.org/10.1021/jp5011549](https://doi.org/10.1021/jp5011549)
Mass-Transport Characteristics of Oxygen at Pt/Anion Exchange Ionomer Interface
Prashant Subhas Khadke and Ulrike Krewer*
- 11224 [dx.doi.org/10.1021/jp501323p](https://doi.org/10.1021/jp501323p)
Nanomorphology Evolution of P3HT/PCBM Blends during Solution-Processing from Coarse-Grained Molecular Simulations
Cheng-Kuang Lee and Chun-Wei Pao*
- 11234 [dx.doi.org/10.1021/jp502004c](https://doi.org/10.1021/jp502004c)
High Rate Capability and Long Cycle Stability of $\text{Co}_3\text{O}_4/\text{CoFe}_2\text{O}_4$ Nanocomposite as an Anode Material for High-Performance Secondary Lithium Ion Batteries
Alok Kumar Rai, Jihyeon Gim, Trang Vu Thi, Docheon Ahn, Sung June Cho, and Jaekook Kim*
- 11244 [dx.doi.org/10.1021/jp502144u](https://doi.org/10.1021/jp502144u)
Alkali Metal Hydride Modification on Hydrazine Borane for Improved Dehydrogenation
Yong Shen Chua,* Qijun Pei, Xiaohua Ju, Wei Zhou, Terrence J. Udovic, Guotao Wu, Zhitao Xiong, Ping Chen,* and Hui Wu*
- 11252 [dx.doi.org/10.1021/jp503127m](https://doi.org/10.1021/jp503127m)
Low-Temperature Reversible Hydrogen Storage Properties of LiBH_4 : A Synergetic Effect of Nanoconfinement and Nanocatalysis
Jie Shao, Xuezhang Xiao, Xiulin Fan, Liuting Zhang, Shouquan Li, Hongwei Ge, Qidong Wang, and Lixin Chen*
- 11261 [dx.doi.org/10.1021/jp503119n](https://doi.org/10.1021/jp503119n)
Impact of Plasma-Induced Surface Damage on the Photoelectrochemical Properties of GaN Pillars Fabricated by Dry Etching
Wei-Jhih Tseng,* D. H. van Dorp, R. R. Lieten, P. M. Vereecken, R. Langer, and G. Borghs
- 11267 [dx.doi.org/10.1021/jp503244c](https://doi.org/10.1021/jp503244c)
Electronics, Vacancies, Optical Properties, and Band Engineering of Red Photocatalyst SrNbO_3 : A Computational Investigation
Chenghua Sun* and Debra J. Searles
- 11271 [dx.doi.org/10.1021/jp503437b](https://doi.org/10.1021/jp503437b)
Efficient "Warm-White" OLEDs Based on the Phosphorescent bis-Cyclometalated iridium(III) Complex
V. Cherpak, P. Stakhira, B. Minaev, G. Baryshnikov, E. Stromylo, I. Helzhynskyy, M. Chapran, D. Volyniuk, D. Tomkutė-Lukšienė, T. Malinauskas, V. Getautis, A. Tomkeviciene, J. Simokaitiene, and J.V. Grazulevicius*
- 11279 [dx.doi.org/10.1021/jp503743e](https://doi.org/10.1021/jp503743e)
Photon Up-Conversion with Lanthanide-Doped Oxide Particles for Solar H_2 Generation
Francisco Gonell, Marta Haro, Rafael S. Sánchez, Patricia Negro, Iván Mora-Seró, Juan Bisquert, Beatriz Julián-López,* and Sixto Gimenez*

- 11285  [dx.doi.org/10.1021/jp5040097](https://doi.org/10.1021/jp5040097)
Performance Improvements in Polymer Nanofiber/Fullerene Solar Cells with External Electric Field Treatment
Ankur Solanki, Bo Wu, Teddy Salim, Edwin Kok Lee Yeow, Yeng Ming Lam, and Tze Chien Sum*
- Surfaces, Interfaces, Porous Materials, and Catalysis**
- 11292  [dx.doi.org/10.1021/jp4120139](https://doi.org/10.1021/jp4120139)
Catalyzed SnO₂ Thin Films: Theoretical and Experimental Insights into Fabrication and Electrocatalytic Properties
A. Rabis, D. Kramer,* E. Fabbri,* M. Worsdale, R. Kötz, and T. J. Schmidt
- 11303 [dx.doi.org/10.1021/jp4120578](https://doi.org/10.1021/jp4120578)
DFT Study of Atomically-Modified Alkali-Earth Metal Oxide Films on Tungsten
Sharon H. Chou, Johannes Voss, Aleksandra Vojvodic, Roger T. Howe, and Frank Abild-Pedersen*
- 11310  [dx.doi.org/10.1021/jp5002012](https://doi.org/10.1021/jp5002012)
Nucleation of Methane Hydrates at Moderate Subcooling by Molecular Dynamics Simulations
Felipe Jiménez-Ángeles and Abbas Firoozabadi*
- 11319 [dx.doi.org/10.1021/jp500909x](https://doi.org/10.1021/jp500909x)
Temperature-Dependent Evolution of the Molecular Configuration of Oxo-Tungsten(VI) Species Deposited on the Surface of Titania
Antonios Tribalis, George D. Panagiotou, George Tsilomelekis, Angelos G. Kalampounias, Kyriakos Bourikas, Christos Kordulis, Soghomon Boghosian,* and Alexis Lycourghiotis
- 11333 [dx.doi.org/10.1021/jp501098v](https://doi.org/10.1021/jp501098v)
Thermal Decomposition of Thin Methanol Films on Deoxygenated Vanadium
Ryutaro Souda*
- 11340 [dx.doi.org/10.1021/jp501208q](https://doi.org/10.1021/jp501208q)
Reaction Pathways of Propanal and 1-Propanol on Fe/Ni(111) and Cu/Ni(111) Bimetallic Surfaces
MyatNoeZin Myint, Yushan Yan,* and Jingguang G. Chen*
- 11350 [dx.doi.org/10.1021/jp501480x](https://doi.org/10.1021/jp501480x)
Time Evolution of a Cl-Terminated Si Surface at Ambient Conditions
P. Chatterjee and S. Hazra*
- 11357  [dx.doi.org/10.1021/jp502494k](https://doi.org/10.1021/jp502494k)
Interaction with a Gold Surface Reshapes the Free Energy Landscape of Alanine Dipeptide
Luca Bellucci* and Stefano Corni*

11365 

[dx.doi.org/10.1021/jp503449q](https://doi.org/10.1021/jp503449q)

Spectroscopy and Dynamics of YD2-o-C8 in Solution and Interacting with Alumina Nanoparticles Electrode
Maria Rosaria di Nunzio, Boiko Cohen, Shyam Pandey, Shuzi Hayse, Giovanni Piani, and Abderrazzak Douhal*

Plasmonics, Optical Materials, and Hard Matter

11377

[dx.doi.org/10.1021/jp4096562](https://doi.org/10.1021/jp4096562)

Optical and Magnetic Excitations of Metal-Encapsulating Si Cages: A Systematic Study by Time-Dependent Density Functional Theory

Micael J. T. Oliveira,* Paulo V. C. Medeiros, José R. F. Sousa, Fernando Nogueira, and Gueorgui K. Gueorguiev

11385

[dx.doi.org/10.1021/jp412462m](https://doi.org/10.1021/jp412462m)

The Stability, Electronic Structure, and Optical Property of TiO₂ Polymorphs
Tong Zhu and Shang-Peng Gao*

11397

[dx.doi.org/10.1021/jp5015115](https://doi.org/10.1021/jp5015115)

Surface-Enhanced Raman Scattering of 4-Nitrobenzenethiol and 4-Aminobenzenethiol on Silver in Icy Environments at Liquid Nitrogen Temperature

Kwan Kim,* Jeong-Yong Choi, and Kuan Soo Shin*

11404 

[dx.doi.org/10.1021/jp5025872](https://doi.org/10.1021/jp5025872)

Texture and Phase Recognition Analysis of β -NaYF₄ Nanocrystals

Valerio Voliani,* Mauro Gemmi, Laura Frances-Soriano, María González-Béjar, and Julia Pérez-Prieto*

Physical Processes in Nanomaterials and Nanostructures

11409

[dx.doi.org/10.1021/jp411568c](https://doi.org/10.1021/jp411568c)

Investigation of the Photophysical and Electrical Characteristics of CuInS₂ QDs/SWCNT Hybrid Nanostructure


Razi Ahmad, Udit Soni, Ritu Srivastava,* Vidya Nand Singh, Suresh Chand, and Sameer Sapra

11417

[dx.doi.org/10.1021/jp412537d](https://doi.org/10.1021/jp412537d)

Effect of Functional Group Topology of Carbon Nanotubes on Electrophoretic Alignment and Properties of Deposited Layer

Mohammad Mostafa and Soumik Banerjee*

11426 

[dx.doi.org/10.1021/jp5001489](https://doi.org/10.1021/jp5001489)

Magnetism in Dopant-Free Hexagonal CdS Nanorods: Experiments and First-Principles Analysis

Donglin Guo, Hao Hua, Qi Yang, Xiaoyan Li, and Chenguo Hu*

11432

[dx.doi.org/10.1021/jp500190m](https://doi.org/10.1021/jp500190m)

Platinum Nanoparticles as Photoactive Substrates for Mass Spectrometry and Spectroscopy Sensors


Maite Cueto, Mauricio Piedrahita, Carlos Caro, Bruno Martínez-Haya,* Mikel Sanz, Mohamed Ujja, and Marta Castillejo


11440 [dx.doi.org/10.1021/jp501989k](https://doi.org/10.1021/jp501989k)
Effect of Temperature and Nanoparticle Size on Sensor Properties of Nanostructured Tin Dioxide Films
Mortko A. Kozhushner, Leonid I. Trakhtenberg, Valeria L. Bodneva, Tatyana V. Belisheva, Aaron C. Landerville, and Ivan I. Oleynik*

11445 [dx.doi.org/10.1021/jp502457w](https://doi.org/10.1021/jp502457w)
Relation between Distortions in the Oxygen Sublattice and the Local Order of Zr in Nanostructured $\text{ZrO}_2\text{-CeO}_2$ Mixed Oxides
Leandro M. Acuña,* Rodolfo O. Fuentes, Marcia C. A. Fantini, and Diego G. Lamas

11454 [dx.doi.org/10.1021/jp502482c](https://doi.org/10.1021/jp502482c)
Time-Resolved Small-Angle X-ray Scattering Study on the Growth Behavior of Silver Nanoparticles
Shi Yan, Zhonghua Wu,* Hongying Yu, Yu Gong, Yuanyuan Tan, Rong Du, Wen Chen, Xueqing Xing, Guang Mo, Zhongjun Chen, Quan Cai, and Dongbai Sun*

11464  [dx.doi.org/10.1021/jp502529d](https://doi.org/10.1021/jp502529d)
Thermal Activation of a Pure Montmorillonite Clay and Its Reactivity in Cementitious Systems
Nishant Garg and Jørgen Skibsted*

11478  [dx.doi.org/10.1021/jp503166g](https://doi.org/10.1021/jp503166g)
In-Situ Immobilization of Silver Nanoparticles on Self-Assembled Honeycomb-Patterned Films Enables Surface-Enhanced Raman Scattering (SERS) Substrates
Yang Ou, Li-Yang Wang, Liang-Wei Zhu, Ling-Shu Wan,* and Zhi-Kang Xu

11485  [dx.doi.org/10.1021/jp503393x](https://doi.org/10.1021/jp503393x)
Decoration of Fe_3O_4 Base Material with Pd Loaded CdS Nanoparticle for Superior Photocatalytic Efficiency
Ramkrishna Sahoo, Anindita Roy, Chaiti Ray, Chanchal Mondal, Yuichi Negishi, S. M. Yusuf, Anjali Pal, and Tarasankar Pal*