

Top Selected Papers in the Physical Chemistry of Energy Materials 2016–2017

Research on energy materials continues to generate a huge amount of activity. The growth of the community in China is enormous, in terms of the creation of research facilities, endowing of major projects, and hiring of personnel, often rather young scientific experts who obtain starting grants after having spent a successful period of research in other laboratories. Energy materials research also continues to expand at a large rate of growth all over the world. Recently we observed the appearance of a serious number of new scientific journals across a variety of publishers that in many cases become rapidly successful. This is because the supply of papers on energy materials research appears to have no physical limits. We are very conscious that many investigators establish their choices of research strategy considering the demand of the topics in terms of facility of publication, impact, and funding. The attitudes and procedures of scientific journals form an essential piece in the machinery of the scientific system.

The Journal of Physical Chemistry has served the research community as a means to present research results for more than a century. *The Journal of Physical Chemistry Letters* was launched less than a decade ago, but it has rapidly been established as a preferred place for communication of results that are both significant and urgent in the context of the current dominant research topics. *JPCL* has been hugely successful in attracting the best papers broadly across the physical chemistry field. We publish, as best as can be predicted, the papers that provide remarkable new discoveries, deep insights, and influential theories or experiments; work that resolves big questions; or results that will interest a broad readership.

The physical chemistry of energy materials is a fascinating area of research that adapts the principles and tools of fundamental physics and chemistry for the best success in obtaining the useful modification of light and substances toward final practical applications. *JPCL* is highly focused on the scientific understanding of energy materials, the determination of how they can be made, and the knowledge of how they operate functionally. We are interested in the original exploration of materials for energy conversion, storage, and lighting; in the insightful analysis of mechanisms that convert photons to electrical or fuel energy; in contributions that bring clarity and orientation to fields that advance rapidly by observations that turn large data sets from a variety of specific materials into real knowledge about their synthesis and performance; and in robust scientific statement, confirmation, and clarification of competing methodologies and interpretations. Therefore, summarizing the recent publications of energy materials research in our journal can provide a broad view of where the recent research topics have been headed and can give significant guidelines in the conglomerate of many interesting topics and results.

The objective of this Editorial is to provide readers with an ordered account of the recent publications of energy

materials in *JPCL*. The short-term impact of research is probably not the final criteria of success and significance of scientific activity. However, there is no doubt that recent markers of scientific prestige and value are very much based on the immediate impact of the research results over a period of 2–3 years. When a representative set of papers is studied from a general perspective it can provide a useful picture for evaluating the progress of the field.

The procedure to highlight the papers has been to analyze a collection of the 10% most cited papers in the years 2016 and 2017. A number of different topics appeared naturally, providing a classification by consistent areas of activity. All of these papers are displayed by topic in [Table 1](#). The list gives a useful account of the guiding trends and preferred problems and approaches for energy materials research in the recent past. In addition, the scientific contributions with highest citation rate into each topic have been presented in the list of the [virtual issue](#).

Starting with papers on new materials for battery applications, we find contributions in the recent trends in the search for alternatives to the classical lithium intercalation compounds: lithium–air, lithium–sulfur, and sodium–oxygen batteries and a seminal exploration of hybrid perovskites for accommodating lithium in the octahedral structure. Advanced methods of analysis of battery operation include the in operando monitoring of redox reactions by optical imaging and ultraviolet (UV) spectroscopy, the microscopic study of the solid electrolyte interphase (SEI), and the first-principles design and prediction of materials.

Solar energy conversion continues the exploration of semiconductor photoelectrodes and catalysts for water splitting. CO₂ reduction is a complex and demanding reaction. Insights on reaction pathways are necessary to prepare effective electrode materials and catalysts. Organic solar cells had shown some signs of stagnation, but lately increases of the efficiency do come up frequently. Impressive efficiencies of the tandem solar cell have been reported, and new mechanistic studies give a central role to materials other than traditional fullerenes for the electron conductor. The papers in this area address charge separation and recombination at the organic heterojunction and singlet–triplet effects for photon management. The mesoporous quantum dot sensitized solar cells also continue to improve by interface designs that control the amount of charge recombination.

The world of photovoltaic (PV) perovskites is advancing in many directions. On one hand, the standard initial MA–Pb–I composition showed enormous potential for PV application, but it also presented some important drawbacks that have turned out to be very difficult to solve. Therefore, there exist a multitude of approaches in chemical and processing routes,

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Table 1. Most Highly Cited JPCL Papers on Energy Materials Published in 2016 and 2017 Ordered by Topic

title	authors	year	issue	first page	last page	DOI
Batteries, Materials						
Sodium–Oxygen Battery: Steps Toward Reality	Landa-Medrano, Imanol; Li, Chunmei; Ortiz-Vitoriano, Nagore; Ruiz de Larramendi, Idoia; Carrasco, Javier; Rojo, Teofil	2016	7	1161	1166	10.1021/acs.jpcllett.5b02845
Lithium–Air Batteries with Hybrid Electrolytes	He, Ping; Zhang, Tao; Jiang, Jie; Zhou, Haoshen	2016	7	1267	1280	10.1021/acs.jpcllett.6b00080
Understanding the Redox Obstacles in High Sulfur-Loading Li–S Batteries and Design of an Advanced Gel Cathode	Zu, Chenxi; Li, Longjun; Guo, Jianhe; Wang, Shaofei; Fan, Donglei; Manthiram, Arumugam	2016	7	1392	1399	10.1021/acs.jpcllett.6b00429
Mapping the Challenges of Magnesium Battery	Song, Jaehye; Sahadeo, Emily; Noked, Malachi; Lee, Sang Bok	2016	7	1736	1749	10.1021/acs.jpcllett.6b00384
Robust NaO ₂ Electrochemistry in Aprotic Na–O ₂ Batteries Employing Etheral Electrolytes with a Protic Additive	Abate, Iwnetim L.; Thompson, Leslie E.; Kim, Ho-Cheol; Aetukuri, Nagaphani B.	2016	7	2164	2169	10.1021/acs.jpcllett.6b00856
Revealing Charge Transport Mechanisms in Li ₂ S ₂ for Li–Sulfur Batteries	Liu, Zhixiao; Balbuena, Perla B.; Mukherjee, Partha P.	2017	8	1324	1330	10.1021/acs.jpcllett.6b03063
Methylammonium Lead Bromide Perovskite Battery Anodes Reversibly Host High Li-Ion Concentrations	Vicente, Nuria; Garcia-Belmonte, Germa	2017	8	1371	1374	10.1021/acs.jpcllett.7b00189
Batteries, Methods						
Ab Initio Prediction and Characterization of Mo ₂ C Monolayer as Anodes for Lithium-Ion and Sodium-Ion Batteries	Sun, Qilong; Dai, Ying; Ma, Yandong; Jing, Tao; Wei, Wei; Huang, Baibiao	2016	7	937	943	10.1021/acs.jpcllett.6b00171
Controlling Solution-Mediated Reaction Mechanisms of Oxygen Reduction Using Potential and Solvent for Aprotic Lithium–Oxygen Batteries	Kwabi, David G.; Tulodziecki, Michal; Pour, Nir; Iktis, Daniil M.; Thompson, Carl V.; Shao-Horn, Yang	2016	7	1204	1212	10.1021/acs.jpcllett.6b00323
Solvent-Dictated Lithium Sulfur Redox Reactions: An Operando UV–vis Spectroscopic Study	Zou, Qingli; Lu, Yi-Chun	2016	7	1518	1525	10.1021/acs.jpcllett.6b00228
Electric Potential Gradient at the Buried Interface between Lithium-Ion Battery Electrodes and the SEI Observed Using Photoelectron Spectroscopy	Maibach, Julia; Lindgren, Fredrik; Eriksson, Henrik; Edstrom, Kristina; Hahlin, Maria	2016	7	1775	1780	10.1021/acs.jpcllett.6b00391
Li Intercalation into Graphite: Direct Optical Imaging and Cahn–Hilliard Reaction Dynamics	Guo, Yinsheng; Smith, Raymond B.; Yu, Zhonghua; Efetov, Dmitri K.; Wang, Junpu; Kim, Philip; Bazant, Martin Z.; Brus, Louis E.	2016	7	2151	2156	10.1021/acs.jpcllett.6b00625
First-Principles Design of Graphene-Based Active Catalysts for Oxygen Reduction and Evolution Reactions in the Aprotic Li–O ₂ Battery	Kang, Joonhee; Yu, Jong-Sung; Han, Byungchan	2016	7	2803	2808	10.1021/acs.jpcllett.6b01071
Solar Water-Splitting Materials						
Improving Stability and Photoelectrochemical Performance of BiVO ₄ Photoanodes in Basic Media by Adding a ZnFe ₂ O ₄ Layer	Kim, Tae Woo; Choi, Kyoung-Shin	2016	7	447	451	10.1021/acs.jpcllett.5b02774
Inverse Oxide/Metal Catalysts in Fundamental Studies and Practical Applications: A Perspective of Recent Developments	Rodriguez, Jose A.; Liu, Ping; Graciani, Jesus; Senanayake, Sanjaya D.; Grinter, David C.; Stacchiola, Darío; Hrbek, Jan; Fernandez-Sanz, Javier	2016	7	2627	2639	10.1021/acs.jpcllett.6b00499
Electrochemical Surface Interrogation of a MoS ₂ Hydrogen-Evolving Catalyst: In Situ Determination of the Surface Hydride Coverage and the Hydrogen Evolution Kinetics	Ahn, Hyun S.; Bard, Allen J.	2016	7	2748	2752	10.1021/acs.jpcllett.6b01276
Developments of Metal Phosphides as Efficient OER Precatalysts	Dutta, Anirban; Pradhan, Narayan	2017	8	144	152	10.1021/acs.jpcllett.6b02249
CO₂ Reduction						
Formation of Copper Catalysts for CO ₂ Reduction with High Ethylene/Methane Product Ratio Investigated with In Situ X-ray Absorption Spectroscopy	Eilert, Andre; Roberts, F. Sloan; Friebel, Daniel; Nilsson, Anders	2016	7	1466	1470	10.1021/acs.jpcllett.6b00367
Identification of Possible Pathways for C–C Bond Formation during Electrochemical Reduction of CO ₂ : New Theoretical Insights from an Improved Electrochemical Model	Goopaster, Jason D.; Bell, Alexis T.; Head-Gordon, Martin	2016	7	1471	1477	10.1021/acs.jpcllett.6b00358
Subsurface Oxygen in Oxide-Derived Copper Electrocatalysts for Carbon Dioxide Reduction	Eilert, Andre; Cavalca, Filippo; Roberts, F. Sloan; Osterwalder, Juerg; Liu, Chang; Favaro, Marco; Crumlin, Ethan J.; Ogasawara, Hirohito; Friebel, Daniel; Petterson, Lars G. M.; Nilsson, Anders	2017	8	285	290	10.1021/acs.jpcllett.6b02273

Table 1. continued

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CO₂ Reduction Building Blocks for High Performance in Electrocatalytic CO ₂ Reduction: Materials, Optimization Strategies, and Device Engineering	Larrazabal, Gaston O.; Martin, Antonio J.; Perez-Ramirez, Javier	2017	8	3933	3944	10.1021/acs.jpcllett.7b01380
Organic Solar Cells Charge Separation and Recombination at Polymer–Fullerene Heterojunctions: Delocalization and Hybridization Effects	D'Avino, Gabriele; Muccioli, Luca; Olivier, Yoann; Beljonne, David	2016	7	536	540	10.1021/acs.jpcllett.5b02680
Ultrafast Long-Range Charge Separation in Organic Photovoltaics: Promotion by Off-Diagonal Vibronic Couplings and Entropy Increase	Yao, Yao; Xie, Xiaoyu; Ma, Haibo	2016	7	4830	4835	10.1021/acs.jpcllett.6b02400
Slow Singlet Fission Observed in a Polycrystalline Peryleneimide Thin Film	Le, Aaron K.; Bender, Jon A.; Roberts, Sean T.	2016	7	4922	4928	10.1021/acs.jpcllett.6b02320
Evidence for Singlet Fission Driven by Vibronic Coherence in Crystalline Tetracene	Morrison, Adrian F.; Herbert, John M.	2017	8	1442	1448	10.1021/acs.jpcllett.7b00230
Efficient Charge Separation of Cold Charge-Transfer States in Organic Solar Cells Through Incoherent Hopping	Athanasopoulos, Stavros; Tscheuschner, Steffen; Baessler, Heinz; Koehler, Anna	2017	8	2093	2098	10.1021/acs.jpcllett.7b00595
Quantum Dot Solar Cells Charge Recombination Control for High Efficiency Quantum Dot Sensitized Solar Cells	Zhao, Ke; Pan, Zhenxiao; Zhong, Xinhua	2016	7	406	417	10.1021/acs.jpcllett.5b02153
Carbon Counter-Electrode-Based Quantum-Dot-Sensitized Solar Cells with Certified Efficiency Exceeding 11%	Du, Zhonglin; Pan, Zhenxiao; Fabregat-Santiago, Francisco; Zhao, Ke; Long, Donghui; Zhang, Hua; Zhao, Yixin; Zhong, Xinhua; Yu, Jong-Sung; Bisquet, Juan	2016	7	3103	3111	10.1021/acs.jpcllett.6b01356
Nitrogen-Doped Mesoporous Carbons as Counter Electrodes in Quantum Dot Sensitized Solar Cells with a Conversion Efficiency Exceeding 12%	Jiao, Shuang; Du, Jun; Du, Zhonglin; Long, Donghui; Jiang, Wuyou; Pan, Zhenxiao; Li, Yan; Zhong, Xinhua	2017	8	559	564	10.1021/acs.jpcllett.6b02864
Perovskites, Chemistry and Compositions Organohalide Lead Perovskites for Photovoltaic Applications	Yusoff, Abd Rashid bin Mohd; Nazeeruddin, Mohammad Khaja	2016	7	851	866	10.1021/acs.jpcllett.5b02893
How Lead Halide Complex Chemistry Dictates the Composition of Mixed Halide Perovskites	Yoon, Seog Joon; Stamplecoskie, Kevin G.; Kamat, Prashant V.	2016	7	1368	1373	10.1021/acs.jpcllett.6b00433
Stabilization of the Perovskite Phase of Formamidinium Lead Triiodide by Methylammonium, Cs, and/or Rb Doping	Syzgantseva, Olga A.; Saliba, Michael; Gratzel, Michael; Rothlisberger, Ursula	2017	8	1191	1196	10.1021/acs.jpcllett.6b03014
High-Quality (CH ₃ NH ₃) ₂ Bi ₂ I ₆ Film-Based Solar Cells: Pushing Efficiency up to 1.64%	Zhang, Zheng; Li, Xiaowei; Xia, Xiaohong; Wang, Zhuo; Huang, Zhongbing; Lei, Binglong; Gao, Yun	2017	8	4300	4307	10.1021/acs.jpcllett.7b01952
Perovskites, Cesium Cesium Enhances Long-Term Stability of Lead Bromide Perovskite-Based Solar Cells	Kulbak, Michael; Gupta, Satyajit; Kedem, Nir; Levine, Igal; Bendikov, Tatyana; Hodes, Gary; Cahen, David	2016	7	167	172	10.1021/acs.jpcllett.5b02597
Cesium Lead Halide Perovskites with Improved Stability for Tandem Solar Cells	Beal, Rachel E.; Slotcavage, Daniel J.; Leijtens, Tomas; Bowring, Andrea R.; Belisle, Rebecca A.; Nguyen, William H.; Burkhard, George F.; Hoke, Eric T.; McGehee, Michael D.	2016	7	746	751	10.1021/acs.jpcllett.6b00002
Solvent Engineering for Ambient-Air-Processed, Phase-Stable CsPbI ₃ in Perovskite Solar Cells	Luo, Pailfeng; Xia, Wei; Zhou, Shengwen; Sun, Lin; Cheng, Jigui; Xu, Chenxi; Lu, Yingwei	2016	7	3603	3608	10.1021/acs.jpcllett.6b01576
Synthesis and Optical Properties of Lead-Free Cesium Tin Halide Perovskite Quantum Rods with High-Performance Solar Cell Application	Chen, Lin-Jer; Lee, Chia-Rong; Chuang, Yu-Ju; Wu, Zhao-Han; Chen, Chienyi	2016	7	5028	5035	10.1021/acs.jpcllett.6b02344
2D Behaviors of Excitons in Cesium Lead Halide Perovskite Nanoplatelets	Li, Jing; Luo, Laihao; Huang, Hongwen; Ma, Chao; Ye, Zhizhen; Zeng, Jie; He, Haiping	2017	8	1161	1168	10.1021/acs.jpcllett.7b00017
Unveiling the Crystal Formation of Cesium Lead Mixed-Halide Perovskites for Efficient and Stable Solar Cells	Nam, Jae Keun; Jung, Myung Sun; Chai, Sung Uk; Choi, Yung Ji; Kim, Dongho; Park, Jong Hyeok	2017	8	2936	2940	10.1021/acs.jpcllett.7b01067
Room-Temperature Synthesis of Mn-Doped Cesium Lead Halide Quantum Dots with High Mn Substitution Ratio	Zhu, Jingrun; Yang, Xiaoling; Zhu, Yihua; Wang, Yuanwei; Cai, Jin; Shen, Jianhua; Sun, Luyi; Li, Chunzhong	2017	8	4167	4171	10.1021/acs.jpcllett.7b01820

Table 1. continued

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Perovskites, Lead-Free						
Lead-Free Halide Double Perovskites via Heterovalent Substitution of Noble Metals	Volonakis, George; Filip, Marina R.; Haghighirad, Amir Abbas; Sakai, Nobuya; Wenger, Bernard; Snaith, Henry J.; Giustino, Feliciano	2016	7	1254	1259	10.1021/acs.jpcclett.6b00376
Band Gaps of the Lead-Free Halide Double Perovskites $Cs_2BiAgCl_6$ and $Cs_2BiAgBr_6$ from Theory and Experiment	Filip, Marina R.; Hillman, Samuel; Haghighirad, Amir Abbas; Snaith, Henry J.; Giustino, Feliciano	2016	7	2579	2585	10.1021/acs.jpcclett.6b01041
Overcoming Short-Circuit in Lead-Free $CH_3NH_3SnI_3$ Perovskite Solar Cells via Kinetically Controlled Gas-Solid Reaction Film Fabrication Process	Yokoyama, Takamichi; Cao, Duyen H.; Stoumpos, Constantinos C.; Song, Tze-Bin; Sato, Yoshiharu; Aramaki, Shinji; Kanatzidis, Mercouri G.	2016	7	776	782	10.1021/acs.jpcclett.6b00118
$Cs_2InAgCl_6$: A New Lead-Free Halide Double Perovskite with Direct Band Gap	Volonakis, George; Haghighirad, Amir Abbas; Milot, Rebecca L.; Sio, Weng H.; Filip, Marina R.; Wenger, Bernard; Johnston, Michael B.; Herz, Laura M.; Snaith, Henry J.; Giustino, Feliciano	2017	8	772	778	10.1021/acs.jpcclett.6b02682
Route to Stable Lead-Free Double Perovskites with the Electronic Structure of $CH_3NH_3PbI_3$: A Case for Mixed-Cation $[Cs/CH_3NH_3]CH(NH_2)_2InBiBr_6$	Volonakis, George; Haghighirad, Amir Abbas; Snaith, Henry J.; Giustino, Feliciano	2017	8	3917	3924	10.1021/acs.jpcclett.7b01584
Discovery of Pb-Free Perovskite Solar Cells via High-Throughput Simulation on the K Computer	Nakajima, Takahito; Sawada, Keisuke	2017	8	4826	4831	10.1021/acs.jpcclett.7b02203
Perovskites, Nanocrystals						
Charge Carrier Lifetimes Exceeding 15 μ s in Methylammonium Lead Iodide Single Crystals	Bi, Yu; Hutter, Eline M.; Fang, Yanjun; Dong, Qingfeng; Huang, Jinsong; Savenije, Tom J.	2016	7	923	928	10.1021/acs.jpcclett.6b00269
Zero-dimensional Cs_4PbBr_6 Perovskite Nanocrystals	Zhang, Yuhai; Saidaminov, Makhud L.; Dursun, Ibrahim; Yang, Haoze; Murali, Banavoth; Alarousi, Erkki; Yengel, Emre; Alshankiti, Buthainah A.; Bakr, Osman M.; Mohammed, Omar F.	2017	8	961	965	10.1021/acs.jpcclett.7b00105
Direct-Indirect Nature of the Bandgap in Lead-Free Perovskite Nanocrystals	Zhang, Yuhai; Yin, Jun; Parida, Manas R.; Ahmed, Ghada H.; Pan, Jun; Bakr, Osman M.; Bredas, Jean-Luc; Mohammed, Omar F.	2017	8	3173	3177	10.1021/acs.jpcclett.7b01381
Size of the Organic Cation Tunes the Band Gap of Colloidal Organolead Bromide Perovskite Nanocrystals	Mittal, Mona; Jana, Atanu; Sarkar, Sagor; Mahadevan, Priya; Sapra, Sameer	2016	7	3270	3277	10.1021/acs.jpcclett.6b01406
Dynamics of Charged Excitons and Biexcitons in $CsPbBr_3$ Perovskite Nanocrystals Revealed by Femtosecond Transient-Absorption and Single-Dot Luminescence Spectroscopy	Yarita, Naoki; Tahara, Hirokazu; Ihara, Toshiyuki; Kawawaki, Tokuhisa; Sato, Ryota; Saruyama, Masaki; Teranishi, Toshiharu; Kanemitsu, Yoshihiko	2017	8	1413	1418	10.1021/acs.jpcclett.7b00326
Perovskites, Two-Dimensional						
Photovoltaic Properties of Two-Dimensional $(CH_3NH_3)_2Pb(SCN)_2I_2$ Perovskite: A Combined Experimental and Density Functional Theory Study	Xiao, Zewen; Meng, Weiwei; Saparov, Bayrammurad; Duan, Hsin-Sheng; Wan, Changlei; Feng, Chunbao; Liao, Weiqiang; Ke, Weijun; Zhao, Dewei; Wang, Jianbo; Mitzi, David B.; Yan, Yanfa	2016	7	1213	1218	10.1021/acs.jpcclett.6b00248
Mechanism for Broadband White-Light Emission from Two-Dimensional (110) Hybrid Perovskites	Hu, Te; Smith, Matthew D.; Dohner, Emma R.; Sher, Meng-Ju; Wu, Xiaoxi; Tuan Trinh, M.; Fisher, Alan; Corbett, Jeff; Zhu, X.-Y.; Karunadasa, Hemamala L.; Lindenberg, Aaron M.	2016	7	2258	2263	10.1021/acs.jpcclett.6b00793
2D Behaviors of Excitons in Cesium Lead Halide Perovskite Nanoplatelets	Li, Jing; Luo, Lihao; Huang, Hongwen; Ma, Chao; Ye, Zhizhen; Zeng, Jie; He, Haiping	2017	8	1161	1168	10.1021/acs.jpcclett.7b00017
First-Principles Study of Novel Two-Dimensional $(C_4H_9NH_3)_2PbX_4$ Perovskites for Solar Cell Absorbers	Wang, Dai; Wen, Bo; Zhu, Ya-Nan; Tong, Chuan-Jia; Tang, Zhen-Kun; Liu, Li-Min	2017	8	876	883	10.1021/acs.jpcclett.7b00003
Room-Temperature Coherent Optical Phonon in 2D Electronic Spectra of $CH_3NH_3PbI_3$ Perovskite as a Possible Cooling Bottleneck	Monahan, Daniele M.; Guo, Liang; Lin, Jia; Dou, Letian; Yang, Peidong; Fleming, Graham R.	2017	8	3211	3215	10.1021/acs.jpcclett.7b01357
How the Structures and Properties of Two-Dimensional Layered Perovskites $MAPbI_3$ and $CsPbI_3$ Vary with the Number of Layers	Zhang, Lei; Liang, WanZhen	2017	8	1517	1523	10.1021/acs.jpcclett.6b03005
Perovskites, Devices and Stability						
Cesium Lead Halide Perovskites with Improved Stability for Tandem Solar Cells	Beal, Rachel E.; Slotavage, Daniel J.; Leijtens, Tomas; Bowring, Andrea R.; Belisle, Rebecca A.; Nguyen, William H.; Burkhard, George F.; Hoke, Eric T.; McGehee, Michael D.	2016	7	746	751	10.1021/acs.jpcclett.6b00002
Cesium Enhances Long-Term Stability of Lead Bromide Perovskite-Based Solar Cells	Kulbak, Michael; Gupta, Satyajit; Kedem, Nir; Levine, Igal; Bendikov, Tatyana; Hodes, Gary; Cahen, David	2016	7	167	172	10.1021/acs.jpcclett.5b02597
Efficient Monolithic Perovskite/Silicon Tandem Solar Cell with Cell Area >1 cm^2	Werner, Jeremie; Wang, Ching-Hsun; Walter, Arnaud; Fesquet, Luc; Seif, Johannes Peter; De Wolf, Stefan; Niesen, Bjoern; Ballif, Christophe	2016	7	161	166	10.1021/acs.jpcclett.5b02686
Surface and Interface Aspects of Organometal Halide Perovskite Materials and Solar Cells	Ono, Luis K.; Qi, Yabing	2016	7	4764	4794	10.1021/acs.jpcclett.6b01951

Table 1. continued

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Perovskites, Devices and Stability						
Highly Efficient All-Inorganic Planar Heterojunction Perovskite Solar Cells Produced by Thermal Coevaporation of CsI and PbI ₂	Frolova, Lyubov A.; Anokhin, Denis V.; Piriyazev, Alexey A.; Luchkin, Sergey Yu.; Dremova, Nadezhda N.; Stevenson, Keith J.; Troshin, Pavel A.	2017	8	67	72	10.1021/acs.jpcclett.6b02594
Probing the Intrinsic Thermal and Photochemical Stability of Hybrid and Inorganic Lead Halide Perovskites	Akbulatov, Azat F.; Luchkin, Sergey Yu.; Frolova, Lyubov A.; Dremova, Nadezhda N.; Gerasimov, Kirill L.; Zhidkov, Ivan S.; Anokhin, Denis V.; Kurmaev, Ernst Z.; Stevenson, Keith J.; Troshin, Pavel A.	2017	8	1211	1218	10.1021/acs.jpcclett.6b03026
Halide Perovskites for Tandem Solar Cells	Lee, Jin-Wook; Hsteh, Yao-Tsung; De Marco, Nicholas; Bae, Sang-Hoon; Han, Qifeng; Yang, Yang	2017	8	1999	2011	10.1021/acs.jpcclett.7b00374
Perovskites, Theory and Computation						
Thermodynamic Origin of Photoinstability in the CH ₃ NH ₃ Pb(1-x)Br _x Hybrid Halide Perovskite Alloy	Brivio, Federico; Caetano, Clovis; Walsh, Aron	2016	7	1083	1087	10.1021/acs.jpcclett.6b00226
Dynamical Origin of the Rashba Effect in Organohalide Lead Perovskites: A Key to Suppressed Carrier Recombination in Perovskite Solar Cells?	Etienne, Thibaud; Mosconi, Edoardo; De Angelis, Filippo	2016	7	1638	1645	10.1021/acs.jpcclett.6b00564
Band Gaps of the Lead-Free Halide Double Perovskites Cs ₂ BiAgCl ₆ and Cs ₂ BiAgBr ₆ from Theory and Experiment	Filip, Marina R.; Hillman, Samuel; Haghighirad, Amir Abbas; Snaith, Henry J.; Giustino, Feliciano	2016	7	2579	2585	10.1021/acs.jpcclett.6b01041
Valence and Conduction Band Densities of States of Metal Halide Perovskites: A Combined Experimental–Theoretical Study	Endres, James; Egger, David A.; Kulbak, Michael; Kerner, Ross A.; Zhao, Lianfeng; Silver, Scott H.; Hodes, Gary; Rand, Barry P.; Cahen, David; Kronik, Leeor; Kahn, Antoine	2016	7	2722	2729	10.1021/acs.jpcclett.6b00946
High Defect Tolerance in Lead Halide Perovskite CsPbBr ₃	Kang, Jun; Wang, Lin-Wang	2017	8	489	493	10.1021/acs.jpcclett.6b02800
Cs ₂ InAgCl ₆ : A New Lead-Free Halide Double Perovskite with Direct Band Gap	Volonakis, George; Haghighirad, Amir Abbas; Miliot, Rebecca L.; Sio, Weng H.; Filip, Marina R.; Wenger, Bernard; Johnston, Michael B.; Herz, Laura M.; Snaith, Henry J.; Giustino, Feliciano	2017	8	772	778	10.1021/acs.jpcclett.6b02682
First-Principles Study of Novel Two-Dimensional (C ₄ H ₉ NH ₃) ₂ PbX ₄ Perovskites for Solar Cell Absorbers	Wang, Da; Wen, Bo; Zhu, Ya-Nan; Tong, Chuan-Jia; Tang, Zhen-Kun; Liu, Li-Min	2017	8	876	883	10.1021/acs.jpcclett.7b00003
Rashba Band Splitting in Organohalide Lead Perovskites: Bulk and Surface Effects	Mosconi, Edoardo; Etienne, Thibaud; De Angelis, Filippo	2017	8	2247	2252	10.1021/acs.jpcclett.7b00328
Structural Instabilities Related to Highly Anharmonic Phonons in Halide Perovskites	Marronnier, Arthur; Lee, Heejae; Geffroy, Bernard; Even, Jacky; Bonnassieux, Yvan; Roma, Guido	2017	8	2659	2665	10.1021/acs.jpcclett.7b00807
Direct-Indirect Nature of the Bandgap in Lead-Free Perovskite Nanocrystals	Zhang, Yuhai; Yin, Jun; Panida, Manas R.; Ahmed, Ghada H.; Pan, Jun; Bakr, Osman M.; Bredas, Jean-Luc; Mohammed, Omar F.	2017	8	3173	3177	10.1021/acs.jpcclett.7b01381
Discovery of Pb-Free Perovskite Solar Cells via High-Throughput Simulation on the K Computer	Nakajima, Takahito; Sawada, Keisuke	2017	8	4826	4831	10.1021/acs.jpcclett.7b02203
Perovskites, Fundamental Properties						
Phonon Mode Transformation Across the Orthorhombic-Tetragonal Phase Transition in a Lead Iodide Perovskite CH ₃ NH ₃ PbI ₃ : A Terahertz Time-Domain Spectroscopy Approach	La-o-vorakiat, Chan; Xia, Huanxin; Kadro, Jeannette; Salim, Teddy; Zhao, Daming; Ahmed, Towfiq; Lam, Yeng Ming; Zhu, Jian-Xin; Marcus, Rudolph A.; Michel-Beyerle, Maria-Elisabeth; Chia, Elbert E. M.	2016	7	1	6	10.1021/acs.jpcclett.5b02223
Octahedral Rotation Preferences in Perovskite Iodides and Bromides	Young, Joshua; Rondinelli, James M.	2016	7	918	922	10.1021/acs.jpcclett.6b00094
Valence and Conduction Band Densities of States of Metal Halide Perovskites: A Combined Experimental–Theoretical Study	Endres, James; Egger, David A.; Kulbak, Michael; Kerner, Ross A.; Zhao, Lianfeng; Silver, Scott H.; Hodes, Gary; Rand, Barry P.; Cahen, David; Kronik, Leeor; Kahn, Antoine	2016	7	2722	2729	10.1021/acs.jpcclett.6b00946
Electron–Rotor Interaction in Organic–Inorganic Lead Iodide Perovskites Discovered by Isotope Effects	Gong, Jue; Yang, Mengjun; Ma, Xiangchao; Schaller, Richard D.; Liu, Gang; Kong, Lingping; Yang, Ye; Beard, Matthew C.; Lesslie, Michael; Dai, Ying; Huang, Baibiao; Zhu, Kai; Xu, Tao	2016	7	2879	2887	10.1021/acs.jpcclett.6b01199
Elastic Constants, Optical Phonons, and Molecular Relaxations in the High Temperature Plastic Phase of the CH ₃ NH ₃ PbBr ₃ Hybrid Perovskite	Létoublon, Antoine; Paofai, Serge; Ruffie, Benoit; Bourges, Philippe; Hehlen, Bernard; Michel, Thierry; Ecolivet, Claude; Durand, Olivier; Cordier, Stephane; Katan, Claudine; Even, Jacky	2016	7	3776	3784	10.1021/acs.jpcclett.6b01709
Direct Experimental Evidence for Photoinduced Strong-Coupling Polarons in Organolead Halide Perovskite Nanoparticles	Zheng, Kaibo; Abdellah, Mohamed; Zhu, Qiusi; Kong, Qingyu; Jennings, Guy; Kurtz, Charles A.; Messing, Maria E.; Niu, Yuran; Goszola, David J.; Al-Marr, Mohammed J.; Zhang, Xiaoyi; Pullerits, Tomu; Cantan, Sophie E.	2016	7	4535	4539	10.1021/acs.jpcclett.6b02046
Temperature Dependence of the Energy Levels of Methylammonium Lead Iodide Perovskite from First-Principles	Saidi, Wissam A.; Ponce, Samuel; Monserrat, Bartomeu	2016	7	5247	5252	10.1021/acs.jpcclett.6b02560

Table 1. continued

title	authors	year	issue	first page	last page	DOI
Perovskites, Fundamental Properties						
Enhanced Optoelectronic Performance on the (110) Lattice Plane of an MAPbBr ₃ Single Crystal	Zuo, Zhiyuan; Ding, Jianxu; Zhao, Ying; Du, Songjie; Li, Yongfu; Zhan, Xiaoyuan; Cui, Hongzhi	2017	8	684	689	10.1021/acs.jpcllett.6b02812
Rashba Band Splitting in Organohalide Lead Perovskites: Bulk and Surface Effects	Mosconi, Edoardo; Etienne, Thibaud; De Angelis, Filippo	2017	8	2247	2252	10.1021/acs.jpcllett.7b00328
Structural Instabilities Related to Highly Anharmonic Phonons in Halide Perovskites	Marronnier, Arthur; Lee, Heejae; Geffroy, Bernard; Even, Jacky; Bonnassieux, Yvan; Roma, Guido	2017	8	2659	2665	10.1021/acs.jpcllett.7b00807
Photoinduced Single- and Multiple-Electron Dynamics Processes Enhanced by Quantum Confinement in Lead Halide Perovskite Quantum Dots	Vogel, Dayton J.; Kryjevski, Andrei; Inerbaev, Talgat; Kilin, Dmitri S.	2017	8	3032	3039	10.1021/acs.jpcllett.6b03048
Long-Lived Photoinduced Polarons in Organohalide Perovskites	Ivanovska, Tanja; Dionigi, Chiara; Mosconi, Edoardo; De Angelis, Filippo; Liscio, Fabiola; Morandi, Vittorio; Ruani, Giampiero	2017	8	3081	3086	10.1021/acs.jpcllett.7b01156
Room-Temperature Coherent Optical Phonon in 2D Electronic Spectra of CH ₃ NH ₃ PbI ₃ Perovskite as a Possible Cooling Bottleneck	Monahan, Daniele M.; Guo, Liang; Lin, Jia; Dou, Letian; Yang, Peidong; Fleming, Graham R.	2017	8	3211	3215	10.1021/acs.jpcllett.7b01357
Temperature-Induced Large Broadening and Blue Shift in the Electronic Band Structure and Optical Absorption of Methylammonium Lead Iodide Perovskite	Yang, Jia-Yue; Hu, Ming	2017	8	3720	3725	10.1021/acs.jpcllett.7b01719
Perovskites, Defects and Dopants						
Heterovalent Dopant Incorporation for Bandgap and Type Engineering of Perovskite Crystals	Abdelhady, Ahmed L.; Saidaminov, Makhsud I.; Murali, Banavoth; Adinolfi, Valerio; Voznyy, Oleksandr; Katsiev, Khabiboullakh; Alarousu, Ekké; Comin, Riccardo; Dursun, Ibrahim; Sinatra, Lutfan; Sargent, Edward H.; Mohammed, Omar F.; Bakr, Osman M.	2016	7	295	301	10.1021/acs.jpcllett.5b02681
Spatially Nonuniform Trap State Densities in Solution-Processed Hybrid Perovskite Thin Films	Draguta, Sergiu; Thakur, Siddharath; Morozov, Yurii V.; Wang, Yuanxing; Manser, Joseph S.; Kamat, Prashant V.; Kuro, Masaru	2016	7	715	721	10.1021/acs.jpcllett.5b02888
Thermally Activated Point Defect Diffusion in Methylammonium Lead Trihalide: Anisotropic and Ultrahigh Mobility of Iodine	Delugas, P.; Cadedo, C.; Filippetti, A.; Mattoni, A.	2016	7	2356	2361	10.1021/acs.jpcllett.6b00963
Band Gap Tuning and Defect Tolerance of Atomically Thin Two-Dimensional Organic-Inorganic Halide Perovskites	Pandey, Mohanish; Jacobsen, Karsten W.; Thygesen, Kristian S.	2016	7	4346	4352	10.1021/acs.jpcllett.6b01998
High Defect Tolerance in Lead Halide Perovskite CsPbBr ₃	Kang, Jun; Wang, Lin-Wang	2017	8	489	493	10.1021/acs.jpcllett.6b02800
Perovskites, Transport and Recombination						
Charge Carrier Lifetimes Exceeding 15 μs in Methylammonium Lead Iodide Single Crystals	Bi, Yu; Hutter, Eline M.; Fang, Yanjun; Dong, Qingfeng; Huang, Jinsong; Savenije, Tom J.	2016	7	923	928	10.1021/acs.jpcllett.6b00269
Radiative Monomolecular Recombination Boosts Amplified Spontaneous Emission in HC(NH ₂) ₂ SnI ₃ Perovskite Films	Milot, Rebecca L.; Eperon, Giles E.; Green, Thomas; Snaith, Henry J.; Johnston, Michael B.; Herz, Laura M.	2016	7	4178	4184	10.1021/acs.jpcllett.6b02030
Surface Recombination and Collection Efficiency in Perovskite Solar Cells from Impedance Analysis	Zarazu, Isaac; Han, Guifang; Boix, Pablo P.; Mhaisalkar, Subodh; Fabregat-Santiago, Francisco; Mora-Sero, Ivan; Bisquert, Juan; Garcia-Belmonte, Germa	2016	7	5105	5113	10.1021/acs.jpcllett.6b02193
Mobility-Lifetime Products in MAPbI ₃ Films	Levine, Igal; Gupta, Satyajit; Brenner, Thomas M.; Azulay, Doron; Millo, Oded; Hodes, Gary; Cahen, David; Balberg, Isaac	2016	7	5219	5226	10.1021/acs.jpcllett.6b02287
Photoresponse of CsPbBr ₃ and Cs ₄ PbBr ₆ Perovskite Single Crystals	Cha, Ji-Hyun; Han, Jae Hoon; Yin, Wenping; Park, Cheolwoo; Ahn, Tae Kyu; Cho, Jeong Ho; Jung, Duk-Young	2017	8	565	570	10.1021/acs.jpcllett.6b02763
Decreasing Radiative Recombination Coefficients via an Indirect Band Gap in Lead Halide Perovskites	Kirchartz, Thomas; Rau, Uwe	2017	8	1265	1271	10.1021/acs.jpcllett.7b00236
Correlation between Photoluminescence and Carrier Transport and a Simple In Situ Passivation Method for High-Bandgap Hybrid Perovskites	Stoddard, Ryan J.; Eickemeyer, Felix T.; Katahara, John K.; Hillhouse, Hugh W.	2017	8	3289	3298	10.1021/acs.jpcllett.7b01185

Table 1. continued

title	authors	year	issue	first page	last page	DOI
Perovskites, Excitons						
Free Carriers versus Excitons in $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite Thin Films at Low Temperatures: Charge Transfer from the Orthorhombic Phase to the Tetragonal Phase	Phuong, Le Quang; Yamada, Yasuhiro; Nagai, Masaya; Maruyama, Naoki; Wakamiya, Atsushi; Kanemitsu, Yoshihiko	2016	7	2316	2321	10.1021/acs.jpcclett.6b00781
Observation of Two Triplet-Pair Intermediates in Singlet Exciton Fission	Pensack, Ryan D.; Ostroumov, Evgeny E.; Tilley, Andrew J.; Mazza, Samuel; Grieco, Christopher; Thorely, Karl J.; Asbury, John B.; Seferos, Dwight S.; Anthony, John E.; Scholes, Gregory D.	2016	7	2370	2375	10.1021/acs.jpcclett.6b00947
Unraveling Triplet Excitons Photophysics in Hyper-Cross-Linked Polymeric Nanoparticles: Toward the Next Generation of Solid-State Upconverting Materials	Monguzzi, Angelo; Mauri, Michele; Frigoli, Michel; Pedrini, Jacopo; Simonutti, Roberto; Larpent, Chantal; Vaccaro, Gianfranco; Sassi, Mauro; Meinardi, Francesco	2016	7	2779	2785	10.1021/acs.jpcclett.6b01115
Free Excitons and Exciton-Phonon Coupling in $\text{CH}_3\text{NH}_3\text{PbI}_3$ Single Crystals Revealed by Photocurrent and Photoluminescence Measurements at Low Temperatures	Phuong, Le Quang; Nakaïke, Yumi; Wakamiya, Atsushi; Kanemitsu, Yoshihiko	2016	7	4905	4910	10.1021/acs.jpcclett.6b02432
Dynamics of Charged Excitons and Biexcitons in CsPbBr_3 Perovskite Nanocrystals Revealed by Femtosecond Transient-Absorption and Single-Dot Luminescence Spectroscopy	Yarita, Naoki; Tahara, Hirokazu; Ihara, Toshiyuki; Kawawaki, Tokuhisa; Sato, Ryota; Saruyama, Masaki; Teranishi, Toshihiko; Kanemitsu, Yoshihiko	2017	8	1413	1418	10.1021/acs.jpcclett.7b00326
Unraveling the Exciton Binding Energy and the Dielectric Constant in Single-Crystal Methylammonium Lead Triiodide Perovskite	Yang, Zhuo; Surrente, Alessandro; Galkowski, Krzysztof; Bruyant, Nicolas; Maude, Duncan K.; Haghighirad, Amir Abbas; Snaith, Henry J.; Plochocka, Paulina; Nicholas, Robin J.	2017	8	1851	1855	10.1021/acs.jpcclett.7b00524
Perovskites, Hysteresis and Ion Migration						
Light-Induced Space-Charge Accumulation Zone as Photovoltaic Mechanism in Perovskite Solar Cells	Zarazua, Isaac; Bisquert, Juan; Garcia-Belmonte, Gemma	2016	7	525	528	10.1021/acs.jpcclett.5b02810
Degradation of Methylammonium Lead Iodide Perovskite Structures through Light and Electron Beam Driven Ion Migration	Yuan, Haifeng; Debroye, Elke; Janssen, Kris; Naiki, Hiroyuki; Steuwe, Christian; Lu, Gang; Morris, Michele; Orgiu, Emanuele; Uji-i, Hiroshi; De Schryver, Frans; Samori, Paolo; Hofkens, Johan; Roelofs, Maarten	2016	7	561	566	10.1021/acs.jpcclett.5b02828
Origin of $J-V$ Hysteresis in Perovskite Solar Cells	Chen, Bo; Yang, Mengjin; Priya, Shashank; Zhu, Kai	2016	7	905	917	10.1021/acs.jpcclett.6b00215
Surface Polarization Model for the Dynamic Hysteresis of Perovskite Solar Cells	Ravishanker, Sandheep; Almorá, Osbel; Echeverría-Arondo, Carlos; Ghahremanirad, Elhaz; Aranda, Clara; Guerrero, Antonio; Fabregat-Santiago, Francisco; Zaban, Arie; Garcia-Belmonte, Gemma; Bisquert, Juan	2017	8	915	921	10.1021/acs.jpcclett.7b00045
Inductive Loop in the Impedance Response of Perovskite Solar Cells Explained by Surface Polarization Model	Ghahremanirad, Elhaz; Bou, Agustín; Olyae, Saeed; Bisquert, Juan	2017	8	1402	1406	10.1021/acs.jpcclett.7b00415
Inverted Hysteresis in $\text{CH}_3\text{NH}_3\text{PbI}_3$ Solar Cells: Role of Stoichiometry and Band Alignment	Shen, Heping; Jacobs, Daniel A.; Wu, Yiliang; Duong, The; Peng, Jun; Wen, Xiaoming; Fu, Xiao; Karuturi, Siva K.; White, Thomas P.; Weber, Klaus; Catchpole, Kylie R.	2017	8	2672	2680	10.1021/acs.jpcclett.7b00571
Metal Halide Perovskites as Mixed Electronic-Ionic Conductors: Challenges and Opportunities—From Hysteresis to Memristivity	Tress, Wolfgang	2017	8	3106	3114	10.1021/acs.jpcclett.7b00975
Light-Independent Ionic Transport in Inorganic Perovskite and Ultrastable Cs-Based Perovskite Solar Cells	Zhou, Wenke; Zhao, Yicheng; Zhou, Xu; Fu, Rui; Li, Qi; Zhao, Yao; Liu, Kathui; Yu, Dapeng; Zhao, Qing	2017	8	4122	4128	10.1021/acs.jpcclett.7b01851
Perovskites under Pressure						
Pressure-Induced Structural and Optical Properties of Organometal Halide Perovskite-Based Formamidinium Lead Bromide	Wang, Lingrui; Wang, Kai; Zou, Bo	2016	7	2556	2562	10.1021/acs.jpcclett.6b00999
Mechanism of Pressure-Induced Phase Transitions, Amorphization, and Absorption-Edge Shift in Photovoltaic Methylammonium Lead Iodide	Szafranski, Marek; Katrusiak, Andrzej	2016	7	3458	3466	10.1021/acs.jpcclett.6b01648
Pressure-Induced Structural Evolution and Band Gap Shifts of Organometal Halide Perovskite-Based Methylammonium Lead Chloride	Wang, Lingrui; Wang, Kai; Xiao, Guanjun; Zeng, Qiaoshi; Zou, Bo	2016	7	5273	5279	10.1021/acs.jpcclett.6b02420
Pressure-Induced Polymorphic, Optical, and Electronic Transitions of Formamidinium Lead Iodide Perovskite	Wang, Pan; Guan, Jiwen; Galeschuk, Draven T. K.; Yao, Yansun; He, Cindy F.; Jiang, Shan; Zhang, Sijia; Liu, Ying; Jin, Meiling; Jin, Changqing; Song, Yang	2017	8	2119	2125	10.1021/acs.jpcclett.7b00665
Pressure-Induced Effects in Organic-Inorganic Hybrid Perovskites	Postorino, Paolo; Malavasi, Lorenzo	2017	8	2613	2622	10.1021/acs.jpcclett.7b00347
Pressure-Induced Structural and Optical Properties of Inorganic Halide Perovskite CsPbBr_3	Zhang, Long; Zeng, Qingxin; Wang, Kai	2017	8	3752	3758	10.1021/acs.jpcclett.7b01577

Table 2. Some Upcoming *JPCL* Perspective Collections

organizer(s)	collection title
Emilio J. Juárez-Pérez	The Causes of Degradation of Perovskite Solar Cells
Omar F. Mohammed	Zero-Dimensional Perovskites: Challenges and Unique Applications
Tõnu Pullerits and Kaibo Zheng	Two Dimensions Better for Perovskites?
Thomas Kirchartz	Optics and Photon Management in Metal-Halide Perovskites for Optoelectronic Applications
Bruno Ehrler and Akshay Rao	Excitonic Up- and Down-Conversion
Antonio Guerrero	Perovskite Solar Cells toward Industrial-Scale Methods and High Efficiencies
Leonard Mueller	Enhancing the Sensitivity of Nuclear Magnetic Resonance through Dynamic Nuclear Polarization
Aron Walsh	Phonons in Perovskite Solar Cells: Theory, Observations, and Physical Effects
Jean-Philip Piquemal	Present and Future of Multiscale Methods for Complex Chemical Systems
Luke A. O'Dell and Marc-Antoine Sani	Dynamic Nuclear Polarization: New Frontiers in the Characterization of Materials and Biomolecules by Magnetic Resonance

and they need to be closely related with the resulting physical properties. In this landscape of activity, new and challenging problems, properties, methods, and hypotheses appear all the time, which drive a very lively growth of the field. The recent papers in *JPCL* that we show in Table 1 illustrate very well the main lines of development.

On the part of the synthesis, composition, and structure, there are different approaches that address the central goals: to obtain compounds that are stable, less or non-toxic, and powerful in PV operation. The main strategy for enhanced stability is to remove the organic part using cesium instead. The central way to reduce toxicity is to decrease Pb content (which so far reduces considerably the PV performance).

Because the perovskite structure allows a wide number of elements and compositions to be mixed and still shows the right physical properties, one can do selective fractional compositions in each place of the perovskite structure, for example, to reduce Pb content by including some Sn instead. Thus, combining different cations and anions forms a major method toward high performance and stability. Nowadays it is typical to combine three mixed cations and three mixed anions to obtain the optimal performance. Obviously such combinations open up many possibilities, which are studied in terms of their bandgap and light absorption features, the film morphology, and so on. Another route to obtain effective materials is to investigate multicomponent compounds inspired by the original MAPI perovskite formulation but substantially away from it, such as $\text{Cs}_2\text{InAgCl}_6$ or $(\text{CH}_3\text{NH}_3)_3\text{Bi}_2\text{I}_9$. These new compounds may show rather modest performance initially but could eventually offer new avenues of materials research for robust energy conversion devices. Many have the impression that perovskite solar cells research revealed a new continent of PV-optoelectronic materials with plenty of unexpected combinations that must be found and mapped. Anything stable with a bandgap between 1 and 3 eV could be useful for stand-alone solar cells, tandem solar cells, light generation, UV detectors, or large-voltage electrochemical applications.

Did not you expect perovskites to go nano? They did. On one hand, the reduction of size to the typical quantum dot scale has provided already outstanding results and new properties in terms of long recombination lifetimes, very large luminescent quantum yields, and rather interesting exciton dynamics. In addition, the quantum dots are benign to be assembled into films that are needed for PV and light-emission devices. On the other hand, the homogeneous perovskite can be turned into a layered one, into which molecular organic sheets interrupt a few semiconductor

Table 3. Recent *JPCL* Perspectives on Energy Materials

authors	title	year	vol.	first page	last page	DOI
Galagan, Y.	Perovskite Solar Cells: Toward Industrial-Scale Methods	2018	9	4326	4335	10.1021/acs.jpcllett.8b01356
Braly, I. L.; Stoddard, R. J.; Rajagopal, A.; Jen, A. K. Y.; Hillhouse, H. W.	Photoluminescence and Photoconductivity to Assess Maximum Open-Circuit Voltage and Carrier Transport in Hybrid Perovskites and Other Photovoltaic Materials	2018	9	3779	3792	10.1021/acs.jpcllett.8b01152
Chen, X. H.; Lu, H.P.; Yang, Y.; Beard, M. C.	Excitonic Effects in Methylammonium Lead Halide Perovskites	2018	9	2595	2603	10.1021/acs.jpcllett.8b00526
Chen, Y. N.; Yu, S.; Sun, Y.; Liang, Z. Q.	Phase Engineering in Quasi-2D Ruddlesden–Popper Perovskites	2018	9	2627	2631	10.1021/acs.jpcllett.8b00840
Liu, X. K.; Gao, F.	Organic–Inorganic Hybrid Ruddlesden–Popper Perovskites: An Emerging Paradigm for High-Performance Light-Emitting Diodes	2018	9	2251	2258	10.1021/acs.jpcllett.8b00755
Akkerman, Q. A.; Abdelhady, A. L.; Manna, L.	Zero-Dimensional Cesium Lead Halides: History, Properties, and Challenges	2018	9	2326	2337	10.1021/acs.jpcllett.8b00572
Mcleodo, J. A.; Liu, L. J.	Prospects for Mitigating Intrinsic Organic Decomposition in Methylammonium Lead Triiodide Perovskite	2018	9	2411	2417	10.1021/acs.jpcllett.8b00323
Bishop, J. E.; Routledge, T. J.; Lidzey, D. G.	Advances in Spray-Cast Perovskite Solar Cells	2018	9	1977	1984	10.1021/acs.jpcllett.8b00311
Jimenez-Solano, A.; Galisteo-Lopez, J. F.; Miguez, H.	Absorption and Emission of Light in Optoelectronic Nanomaterials: The Role of the Local Optical Environment	2018	9	2077	2084	10.1021/acs.jpcllett.8b00848
Sun, J.; Yang, J.; Lee, J. I.; Cho, J. H.; Kang, M. S.	Lead-Free Perovskite Nanocrystals for Light-Emitting Devices	2018	9	1573	1583	10.1021/acs.jpcllett.8b00301
Bandyopadhyay, A.; Ghosh, D.; Pati, S. K.	Shining Light on New-Generation Two-Dimensional Materials from a Computational Viewpoint	2018	9	1605	1612	10.1021/acs.jpcllett.8b00044
Straus, D. B.; Kagan, C. R.	Electrons, Excitons, and Phonons in Two-Dimensional Hybrid Perovskites: Connecting Structural, Optical, and Electronic Properties	2018	9	1434	1447	10.1021/acs.jpcllett.8b00201

layers, causing effective carrier confinement. These “two-dimensional” materials display enhanced quantum yields, improved stability, and protection against humidity, and they offer desirable fundamental properties as the bottleneck for hot carrier cooling.

From the point of view of effectiveness of the perovskite solar cell, different aspects of full devices have been addressed. The tandem solar cell is a preferred strategy, normally combined with a highly efficient silicon layer. New routes of preparation like coevaporation are addressed, and the control of interfaces is always a central concern.


Moving toward the insight on microscopic and fundamental properties that cause the observed behavior, we find a variety of important results that have been obtained by first-principles calculation, very often in connection to experimental results presented in the same paper. Thus, we find analysis of the exploration of properties of new appealing compounds, like the evolution of the bandgap and the investigation of the pathways for carrier recombination in terms of carrier density and dynamic properties, often related to specific effects of the perovskite caused by the heavy atom in the center of the octahedron.

Considering a more microscopic level, a number of experimental investigations into fundamental properties appear, such as the evolution of electronic structure, energy levels, and the interactions of carriers with phonons; structural relaxations; and their connection to phase transitions. For decades it has been well-known that the control of foreign atoms and defects in the structure is a major factor for the success of good PV materials. In the perovskite family, the often-used solution-processing methods do not normally help to facilitate lattice purity. Therefore, the presence and effects of defects are being intensively studied. It is well-known that migration of vacancies is facile, with a high impact on device performance. Additionally, the analysis of the role of defects in nonradiative recombination brings new and very important insights. The next block contains studies on carrier transport and recombination, which have a central impact at the device level, like surface and internal nonradiative recombination and the correlations between transport and recombination rates. It is followed by the topic of the study of hot and excited carriers, the formation and persistence of excitons, and their conversion and dynamics. Based on the progress of fundamental insights, it is necessary to establish the dominant factors of operation at the device level. Here features prominently the hysteresis obtained when looping current–voltage curves. The ionic/electronic transport and its impact on surface recombination and capacitance have provided useful insights. Finally, the application of high pressure has been adopted as a popular method to compress the lattice and observe the consequent modification of photophysical properties.

Based on this summary of activities of the previous 2-year period, we suggest that you follow the current developments by periodically reading our page of most accessed Letters, which reveals very well the interests of the community. You can access the weekly updated site here: <https://pubs.acs.org/journal/jpcld>.

In addition, *JPCL* is permanently interested in promoting scientific discussion of the main ongoing topics of research. We have commissioned a series of Perspective collections indicated in [Table 2](#) that will bring a consistent set of short and informative discussions and accounts on specific topics,

especially where the research seems to be crystallizing in new directions. Some recently published Perspectives are shown in [Table 3](#).

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Notes

Views expressed in this editorial are those of the author and not necessarily the views of the ACS.