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Nanostructured Materials for Next-Generation Energy Storage and Conversion

Advanced Battery and Supercapacitors

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With 186 Figures and 23 Tables

Springer

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Preface to Volume III on Batteries

Benjamin Franklin used a battery to describe an array of charged glass plates in 1748 and within 90 years, the advent of electric doorbells, telegraphs, and telephones required a backup energy source. John Daniell (1836) developed primary battery in the form of a cell which could deliver 1.1 V and specific energy less than 0.1 MJ/kg to power these devices and the demand for greater output never ceased. Almost 115 years later, Lew Urry developed (1949) the Alkaline Manganese Battery with 1.25 V and a specific energy around 0.4 MJ/kg. Almost 20 years later (in 1971) Alexandr Kloss and Boris Tsenter implemented nickel and hydrogen to form the precursor of the Nickel Metal Hydride battery, also able to deliver 1.2 V but at a higher specific energy (~140 MJ/kg). Lastly, the work by Akira Yoshino of Asahi Chemical led to the lithium-ion battery at 1.5 V and a specific energy density of 0.8 MJ/kg. This was rapidly followed by the lithium polymer battery which had a flexible casing and enabled the form factor to be altered. Portable electronics could be used for longer periods, including cell phones, laptops, and multimedia devices, such as tablets, ipads, nanoPCs, and wearable electronics, increasing lithium-ion battery sales past the billion units sold mark.

The advantage of the lithium-ion rechargeable batteries as secondary batteries (LIB) relative to nickel-cadmium or nickel-hydride batteries is the endurance of the battery coupled with high specific energy density and no memory effects. These storage devices make up the top three choices, after which manganese dioxide-zinc and lead acid are the next most common storage device. Unlike the other metals, lithium has distinct advantages. It has a low atomic mass, low ionization enthalpy, and high electrode potential, resulting in high energy density relative to zinc-based batteries.

Lithium-ion batteries are a system where the lithium metal forms the anode with a nonaqueous electrolyte such as propylene carbonate-lithium perchlorate and carbon-based cathode. The lithium at the anode forms whisker-like formations which resemble dendrites, causing the battery to short-circuit, in addition to safety issues related to a strong oxidizer such as perchlorate. Other concerns relate to replacement of lithium aluminum and/or polyacene conducting polymer used for memory backup or powering small devices with solar recharge, which may be less efficient and more costly. The “current” lithium-ion batteries do not have lithium metal but intercalation of lithium ions into the active electrode surfaces, using the Asahi design, which uses

the carbon-based anode and lithium cobalt oxide as the cathode. During charging, lithium would be inserted into the carbon anode, and during discharging, lithium would be extracted. The battery design due to conducting polymers could be cylindrical and was 18 mm by 65 mm in length and known as 18650 type with a capacity of 800 mAh/g. During the decades, after World War II, the demands for portable energy have progressively increased, requiring design of a new generation of energy storage devices. Recently, increased battery usage and lifespan have been achieved by the substitution of carbon-based anodes with more flexible graphite-based carbon and changes to electrolyte and modification of lithium cobalt oxides and cell design (polymers, binders, and internal circuitry) relative to lithium only anodes. The early batteries contained mesophase carbon microbead (MCMB with a capacity of 280 mAh/g). By incorporating functional electrolytes that passivate the electrode, higher graphitization of the anode carbon material can be achieved without solvent decomposition, leading to greater catalyticity at the active electrode surface. This graphitization could be accomplished using mesophase carbon fiber, or more active form of MCMBs yielding capacity of 372 $mAh.g^{-1}$. The addition of cyclohexylbenzene would lead to the generation of hydrogen gas at higher voltages and would interrupt the current output, safely shutting down the battery. In the early 2000s, the 18650 type cell had a capacity of 2.4 Ah or an energy density of 200 Wh/kg, which currently have increased to 3.6 Ah and $\sim$ 250 Wh/kg. The passivation of the active surfaces through the introduction of electrolyte additives has enabled the higher energy densities to be reached. Thus, a conductive membrane protects the positive active material in a similar manner to the formation of a solid electrolyte interface to protect the anode; comparison is given below:

Primary cell $\rightarrow$	Alkaline	Lithium iron disulfide ($LiFeS_2$)	Lithium manganese dioxide ($LiMnO_2$)
Specific energy (Wh/kg)	200	300	280
Voltage (V)	1.5	1.5	3.3
Continuous voltage output	Low	Intermediate	Intermediate
Passivation layer	No, N/A	Yes, moderate	Yes, moderate
Operating temperature (OT, °C)	$0 < OT < 60$	$0 < OT < 60$	$-30 < OT < 60$
Shelf-life (SL, years)	10	15	$-10 < SL < 20$

Note: The cathode is carbonaceous material and the anode hosts the active material

To achieve even higher capacities, electrode conditioning is required. Here the cell undergoes several charge-discharge cycles at a low rate (1/4 C) to decompose the additives and form the protective film. The cell is held in their charged state for a week (e.g., 0.005 V vs. Li/Li^+ for 10 h, Li^+ possess ultrahigh capacity [3,860 mAh g^{-1}] and the very low standard negative electrochemical potential [−3.040 V]) to ensure completion of the protective film. In the absence of conditioning, lithium ions can intercalate into graphite (in propylene carbonate-based electrolytes) forming a large number of active sites. These sites are formed because of nonhomogeneous voltage distribution across the anode surface due to underpotential (0 V vs. Li/Li^+) during the Li+ intercalation. Areas of graphite which become exfoliated do not get

Table 1 Summary of the chemistries and configuration of most common secondary battery platforms

Secondary cell →	Lead acid	Ni-Cd	Ni MH	Li cobalt	Li manganese
Specific energy (SE, Wh/kg)	<50	<80	<120	150 < SE < 250	100 < SE < 150
Shelf-life at 80% depth of discharge (cycles)	300	1,000	500	1,000	1,000
Cell voltage (V)	2	1.2	1.2	3.6	3.7
Columbic efficiency (CE, %)	90	90	90	99	99
Decade or year introduced	The 1880s	The 1950s	1970–1990	1991	1996
Time to charge (h)	16	2	4	2	2
Operating charge temperature (OT, °C)	−20 < OT < 50	0 < OT < 45	0 < OT < 45	0 < OT < 45	0 < OT < 45

Note the charge and discharge temperature(s) are different; typically the battery can discharge at lower temperatures but should not be charged if frozen. Cycle life is based on the depth of discharge (DoD), where shallow DoD at moderate to cool temperatures will prolong cycle life.

Li^+ penetration, instead Li metal deposition occurs. This would decrease cell potential to 0.8 V and decrease the cell life cycle. The next stage of development for the 18650 type cells is the use of graphene, planar lithium-nickel-cobalt-aluminum, and nickel-manganese-cobalt cathode-type materials, in addition to new electrolyte additives to promote Li^+ intercalation, suppress Li metal deposition, and promote greater homogeneity across the electrode surface. With these advances, a capacity of 3.0 Ah may be possible by focusing on nano-carbonaceous materials, improved Li^+ intercalation, and use of polyanions other than oxides to increase cell voltages. These different chemistries and formulations are summarized in Table 1.

This book contains an overview of energy policy. Energy policy is critical to long-term planning and stability. While consumer demands related to home and travel account for 4% of the gross domestic product, they account for 28% and 41% of energy usage and CO_2 emissions, respectively. Electrical storage such as LIBs has a CO_2 "tax" associated with them. Only hydroelectric is CO_2-neutral, although fuel cells could fall into this category, LIB, in the long run, could assist in lowering the CO_2 emission profile when compared with electrical generation using coal (baseline comparison), which has been subjected to peak-load pricing and lead to increasing the efficiency of national energy resources, clean-coal development, as well as

development of sustainable resources. Lithium-ion batteries have a role to play both as portable power and as storage, where electric vehicles could be used to power homes in emergencies such as earthquakes and hurricanes when the "centralized grid" fails. The role of national energy policy vis-à-vis LIB and energy storage including recycling of lithium-ion batteries are reviewed.

Other chapters are more traditional in offering an in-depth review of electrode materials, electrolytes, and additives for LIB, as well as indicators of the future directions for continued maturation of the LIB. Here, the authors will explicitly discuss advances in electrode design as the anatomy of the battery is the same as in Daniell's time of anode, cathode, electrolyte, and casing/binding. The authors discuss materials composites for forming newer more reactive electrode surfaces without side reactions or dendrite formation, with higher specific capacity, energy densities, and cycling stability. The fabrication using more streamlined procedures where appropriate is discussed, including newer materials, such as antimony trioxide, chalcogens, and titanium/molybdenum disulfide as high potential anodes. Cathode materials based on nickel cobalt manganese oxide have been employed to minimize cation dissolution of the cathode materials. Other approaches include the use of layered oxides, structured materials to encapsulation designed to reduce the degree of material dissociation, particularly after prolonged use. In addition, alternative strategies related to modification of carbon nanotubes, graphite, and graphene with dopants, passivation of electrodes by coating, or alloying to enhance Li-ion diffusivity are explored. The purposes of such strategies and approaches are to minimize lithium metal deposition and to improve electrode conductivity, ionic mobility, and battery capacity during charging and discharging cycles and use.

All-solid-state lithium-ion batteries' solid electrolytes, such as NASICON-type, perovskite-type, anti-perovskite type, garnet-type, sulfide-type, Li_3N-type, and other chemistries, require optimal ionic conductivity and electrochemical stability at room and higher operational temperatures. These performance characteristics are discussed with respect to changes in ion mobility at different temperature regimes. The current challenges related to electrolyte selection, refinement of the interfaces, and interfacial resistance are reviewed beyond LISICON- and LiPON-type of solid electrolytes.

Room temperature molten salts (ionic liquids) have drawn attention for electrochemical energy storage. These systems offer excellent thermal and electrochemical stability, exhibit low volatility, and are enabled as electrolytes in batteries such as LIBs, sodium-ion, lithium-air (O_2), and Li-sulfur batteries for clean energy storage. The issue of low volatility and low flammability is discussed as well as used in all-solid-state batteries to improve the conductivity of the solid electrolyte, in addition to modification of electrode materials to take advantage of the new physical and chemical properties.

The thermochemistry and modeling aspects are also discussed. Lithium-ion batteries' stability is typically evaluated by cycling under a galvanostatic regime ($\sim$1/4 C – C/2-rate) between 2.75 V and 4.2 V for up to 250–1,500 cycles. After each completed 25n (n = 1–4) cycles, the discharge capacity, capacity loss, and average discharge potential are evaluated. Then cells undergo a supplemental charge and

discharge cycle at higher C/6 rate followed by thermodynamics measurements to determine the open-circuit potential (OCP), entropy, and enthalpy values. Calculations show that state functions of entropy and enthalpy exhibit higher sensitivity to morphological changes in the electrode surface or crystal structure, such as graphite carbon-based anodes and lithium cobalt oxide cathode through repeated cycling (aging) relative to changes in Gibbs free energy estimated from the state of charge or depth of discharge, and OCP values.

Coupled with ex situ X-ray diffractometry, electron microscopy, and Raman spectroscopy analyses on the electrode materials, the relationship between state functions, electrochemical output, crystal structure composition, and density of states can be assessed at both the anode and cathode during aging and inferences made using computational means of processes to stabilize the cathode and/or anode by increased graphitization during the aging process.

The role of non-lithium electrodes is also discussed as it is apparent that increased electric vehicle usage will deplete lithium and cobalt unless aggressive recycling, reuse, and transition to non-lithium are introduced at an early stage, as the demand for portable energy is likely to increase in the near term.

The general aim has been to learn how to assess the technical impact of new active materials and to increase charge density as well as operational reliability, cost, ease of use, and safety. Lastly, no book would be complete without the stellar contribution of the authors, their research group, and institutions. We also would like to extend our deep appreciation to our institution, colleagues, and students as well as the editorial staff at Springer who have strived to deliver the best possible scholarly product. As always, errors and omission are the responsibility of the editors, for which we as preface authors ask forgiveness.

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Kingsville, USA
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Nancy KingSanders
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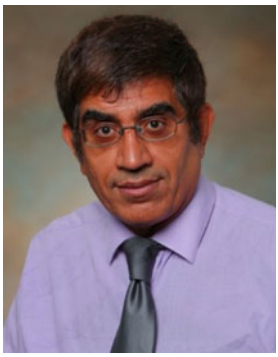
About the Editors

Qiang Zhen received his doctoral degree in the field of Metallurgical Physical Chemistry at the University of Science and Technology Beijing in 2000. Currently, he is a distinguished Professor of Research Center of Nano-Science and Nano-Technology, Shanghai University. He is the Director of Advanced Functional Materials Laboratory, Engineering Research Center of Material Composition and Advanced Dispersion Technology, Ministry of Education, China. He also serves as the Dean of the Science and Technology Development Academy of Shanghai University, is one of the executive members of the China Instrument Functional Materials Society Council, and is member of China Silicate Society. In 2002, he visited the Department of Mechanical Engineering, Hong Kong University, and then the French National Center for Scientific Research, University of Science and Technology in Lille, France, from 2005 to 2012. His research interests focus on solid electrolyte for fuel-cells and sensors, and design, fabrication, and characterization of micro-/nano-composites. He has directed more than 30 scientific research projects, supported by different funding agencies, such as National Natural Science Foundation of China (NSFC), NSFC International Cooperation Plan, and Excellent Talents Supporting Programs. He has published more than 60 papers as a leading coauthor and has reviewed journal papers and project proposals.



Sajid Bashir received his Ph.D. in Analytical Chemistry from the University of Warwick, England, 2001. He was a postgraduate research associate at Cornell University to conduct research in the field of plant genetics. Currently, he is a Full Professor at Texas A&M University-Kingsville (TAMUK) and a Faculty Fellow at the US Air Force. He has directed and participated in more than 20 projects supported by the Welch Foundation, TAMUK, Texas Workforce Commission, and US National Institutes of Health. He has coauthored more than 80 book chapters and peer reviewed journal articles. He is a Fellow and Chartered Chemist of the Royal Society of Chemistry and a Chartered Scientist. During his service in TAMUK, he trained more than 3,000 students on both undergraduate and graduate levels. He created online courses and established safety training protocols in conjunction with the risk management. Currently, he collaborates with the local law enforcement as a consultant.

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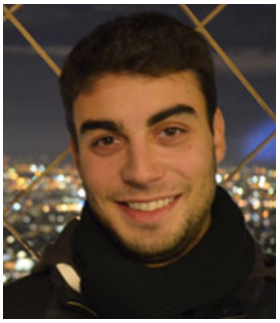
About the Authors

Dr. Nancy KingSanders' background in higher education spans more than 27 years to include a current appointment as Associate Vice President for Student Success at Texas A&M University-Kingsville, a position she has held since 2011. Prior appointments include Associate Dean for Graduate Studies, Administrative Intern for Academic Affairs, Graduate Music Education Coordinator, as well as attaining tenure and the rank of Full Professor in the Music Department at Texas A&M University-Kingsville. Under her administrative leadership at TAMUK, she established the Center for Student Success to include AVID (Advancement Via Individual Determination) for Higher Education, the First-Year Experience, a two-semester First-Year Seminar Course, Centralized Academic Advising, the Graduation Pathway Success Mentoring Center, the Pathway Academic Assistance Tutoring Center, Freshman Interest Groups, Academic Career Literacy, Mapping First-Year Seminar curriculum to General Education Component Area options, and Javelina Common Read Program, resulting in a 15.9% increase in First-Time in College retention at Texas A&M University-Kingsville. She was also selected as a National First-Year Student Advocate by Cengage and the National Resource Center for the First-Year Experience and Students in Transition. Dr. KingSanders' other responsibilities include all academic support for undergraduate students and Co-Principal Investigator for a Title V Individual $2.625 Million Hispanic Serving Institution Grant to embed research into undergraduate courses.

Weixin Song is a Ph.D. student in Materials Science at Imperial College London, United Kingdom. He started his Ph.D. in 2015 funded by the President's Ph.D. Scholarship of Imperial College after he received his B.Sc. in 2012 and M.Sc. in 2015, both from Central South University, China. His research interests are materials electrochemistry and materials characterizations, particularly the applications in energy storage, electrocatalysis, and photoelectrocatalysis. He has 39 publications that have been cited more than 1,700 times and 17 licensed patents. He has been awarded the Armourers and Brasiers Rolls-Royce Scheme in 2018 and the STFC Early Career Award in 2016 from the United Kingdom. He was also awarded the national scholarship and the highest honor when he studied in Central South University. He is a member in Center for Doctoral Training (CDT) in Advanced Characterization of Materials and London Center for Nanotechnology.

Jun Chen is a Ph.D. student in the Department of Materials at the University of Oxford, United Kingdom. She received her Bachelor's degree in Applied Chemistry in 2014 and Master's degree in Physical Chemistry on Metallurgy in 2017, both from Central South University, China. Her Master's research focused on the synthesis, characterization, and electrochemical application of titanium-based nanomaterials for energy storage devices. She was awarded the national scholarship and the honor of "Top Ten Outstanding Students" during her study in Central South University. She then started her Ph.D. in October 2017 in Prof. Jamie Warner's group, fully funded by China Scholarship Council. Her research interest is in two-dimensional (2D) materials, particularly the atomic structure study of transitional metal dichalcogenides and their heterostructures for understanding their properties and behavior. She has 26 publications in peer-reviewed journals, with more than 1,000 citations since 2014, as well as 7 licensed patents.

Carlos M. Costa graduated in Physics in 2005 and obtained his Master's degree in Materials Engineering in 2007. In 2014, he received his Ph.D. in Physics from the Science School of the University of Minho. Currently, he is postdoctoral researcher at the same institution. His work is mainly focused on the development of advanced polymer composites and new materials and formulations for energy storage applications, i.e., lithium-ion batteries and printed batteries.



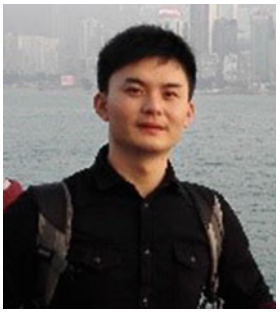
Renato Gonçalves graduated in Chemistry in 2009, in 2011 received his Master's degree in Characterization Techniques and Chemistry Analysis, and in 2017 obtained his Ph.D. in Materials Engineering, all at the University of Minho, Portugal. Currently, he is working with Electroactive Smart Material group of the Physics Department at the University of Minho, Portugal. His work focuses on polymers composites, inorganic synthesis, and magnetoelectric nanocomposites with advanced applications like sensors and actuators. Recently, his work focuses on energy field at innovative green printed batteries for advanced devices. He also collaborated with the University of Basque Country, Spain; BCMaterials, Spain; and Cambridge University, United Kingdom, among others.

S. Lanceros-Méndez graduated in Physics at the University of the Basque Country, Leioa, Spain. He obtained his Ph.D. at the Institute of Physics of the Julius-Maximilians-Universität Würzburg, Germany. He is Ikerbasque Research Professor and Scientific Director at BCMaterials – Basque Center for Materials, Applications and Nanostructures, Leioa, Spain, and Associate Professor at the Physics Department of the University of Minho, Portugal (on leave). His work is focused in the area of smart and multifunctional materials for sensors and actuators, energy, and biomedical applications.

Bin Liu received his Ph.D. from Huazhong University of Science and Technology in China. He is currently a research scientist in the Electrochemical Materials and Systems Group in the Energy Processes & Materials Division at Pacific Northwest National Laboratory. Dr. Liu has extensive experience in the development of electrodes and electrolytes for next-generation energy storage devices (i.e., Li-metal battery, Li-O_2 battery, flexible Li-ion batteries, fiber supercapacitors, Mg-ion battery, and functional integrated devices). Dr. Liu has published 1 book chapter and more than 45 papers with total citations of over 4,200 and H-index of 30. Seven papers were selected as Thomson Reuters ESI 1% Highly Cited Papers. Eight papers were featured as cover and back cover of peer-reviewed journals. His studies were highlighted by American Association for the Advancement of Science (AAAS), *Nature Nanotechnology*, *Nature Photonics*, Materials Research Society (MRS) *Materials360*, weekly Royal Society of Chemistry (RSC) Publishing press pack, Chemie.DE, *Chemistry World*, and China Central Television Channel 1 (CCTV 1). Dr. Liu holds three issued Chinese patents and one pending US patent as well.

Huilin Pan received her Ph.D. in Condensed Matter Physics from the Institute of Physics Chinese Academy of Sciences. She is currently serving as a research scientist in the field of electrochemical materials and systems at Pacific Northwest National Laboratory. Dr. Pan has 8 years of experience in energy storage materials/chemistry and advanced characterizations in different electrochemistry systems, including lithium, sodium, and zinc batteries. She has published more than 30 papers on battery-related research and had filed 4 US patent applications. She was honored as the "TOP 1% author, highly cited in the Royal Society of Chemistry" in 2014. Her primary research interest includes the development of battery materials and electrolytes for energy storage and the underlying reaction mechanisms in battery systems.

Wei Liu received her Bachelor's in Materials Physics from Beijing Normal University in 2008 and Ph.D. in Materials Science and Engineering from Tsinghua University in 2013. During the year 2010–2011, she visited the University of Tokyo for half a year. From 2013 to 2017, she worked at Stanford University as a postdoctoral scholar. She is currently Assistant Professor at ShanghaiTech University. Her research interests cover the area of materials science, nanotechnology, and solid state ionics, with a focus on studies of lithium batteries and fuel cells. Dr. Liu has been an author or coauthor of 47 papers published in journals such as *Nature Energy*, *Nature Communications*, *Science Advances*, *Advanced Materials*, and *Journal of the American Chemical Society*. She is also peer reviewer of journals including *Joule*, *Nano Letters*, and *Nano Energy*. In 2018, she was awarded as one of the Distinguished Young Scholars by the Thousand Talents Program.



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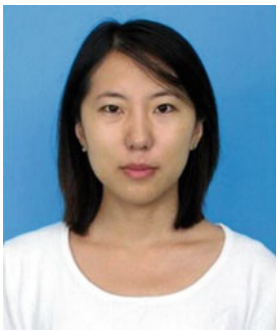
Dr. Yanbin Chen, Professor, candidate of the National Talent Project in China, and candidate of the Beijing Capital Technical Leading Talent Project, is currently the Vice President of Beijing Easpring Material Technology Co., Ltd. He was awarded Ph.D. by the University of Science and Technology Beijing in 2001. He has been engaged in research, development, and industrialization of the key materials for lithium battery for 20 years. Up to now, he has developed more than 50 products of three

series cathode materials, including lithium cobalt oxide, lithium manganese oxide, and lithium nickel cobalt manganese oxide, has published more than 50 papers, has obtained 16 licensed patents, and has drafted 9 national and industrial standards. The Easpring is a global top supplier of cathode materials for lithium-ion batteries, providing high-end products to leading battery makers, including LG Chem, Samsung SDI, SK Innovation, Sanyo, Sony, CATL, Farasis, BYD, BAK, etc. The Easpring has been recognized as an Excellent Export Enterprise, National Technical Innovation Demonstration Enterprise, and National Accredited Enterprise Technical Center.

Professor Yafei Liu is currently the Director of Institute of Lithium-ion Battery Materials of Beijing Easpring Material Technology Co., Ltd. He is also an affiliate with the State Chinese Government Council Special Allowance Program as Topic Expert. He was awarded Ph.D. by the University of Science and Technology of China in 2001. He has been engaged in research, development, and industrialization of lithium-ion cathode materials and their precursors, fuel cell materials, and gas-sensitive and functional materials for a long time. So far, he has published more than 50 papers and has applied 52 patents.

Xiujun Qi received her Bachelor's degree in School of Materials Science and Engineering, Liaocheng University, China, in 2015. She attended China University of Mining and Technology in the same year, pursuing her Ph.D. in School of Materials Science and Engineering under the guidance of Prof. Zhicheng Ju. Her current research focuses on the synthesis and electrochemical characterization of heteroatom-doped carbon materials for advanced batteries such as lithium-ion batteries and potassium-ion batteries. She has coauthored six research articles in peer-reviewed journals and has joined several international conferences.



Zheng Xing received her Bachelor and Master degrees in School of Chemistry and Chemical Engineering from Shandong University, China, in 2007 and 2010, following which she began her Ph.D. at the School of Chemistry and Materials Science at the University of Science and Technology of China under the supervision of Prof. Yitai Qian. She received her Ph.D. in Inorganic Chemistry in June 2013. She then joined the School of Materials Science and Engineering at the China University of Mining and Technology as an Assistant Professor. Her research focuses on the study of the transitional metal oxides and new carbon-based functional materials for energy conversion and storage. She has published more than 30 research articles in peer-reviewed journals and has joined many international conferences.

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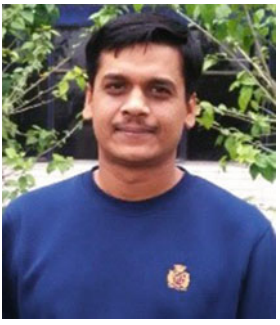
Claudiu B. Bucur obtained his Ph.D. in 2008 from Florida State University under the mentorship of distinguished Leo Mandelkern Professor of Polymer Science, Joseph B. Schlenoff. He studied the manner in which polyelectrolyte multilayers assemble and how doping them with ions changes their mechanical and thermodynamic properties. In 2010, he completed his postdoctoral studies at the USDA Agricultural Research Service Labs, where he investigated corrosion inhibition via biomembranes. Dr. Bucur then joined the Post Lithium

Ion Research Group at the Toyota Research Institute of North America, where he focused on metallic anodes such as magnesium, lithium, sodium, and their electrolytes as well as high capacity conversion cathodes such as the sulfur cathode. He expanded upon his experience with polymers, corrosion, and interfaces and was able to advance many areas in the battery field. Currently, Dr. Bucur is Chief Engineer and Program Director for new battery and solid electrolyte projects at Great Wall Motor, the largest SUV manufacturer in China. He is fascinated by energy storage and dreams of creating the ultimate battery.

Tharamani C. Nagaiah received her Ph.D. in Materials Electrochemistry from Bangalore University, India, in 2005. She joined the Indian Institute of Technology Ropar in 2012 as an Assistant Professor in the Department of Chemistry. Dr. Tharamani has previously worked as a Research Associate at the Indian Institute of Science, Bangalore, and thereafter she moved to the University of Saskatchewan, Canada, as a postdoctoral fellow following which she joined at the Ruhr Universität Bochum, Germany. She has also been a recipient of many prestigious fellowships like Alexander von Humboldt Postdoctoral Fellowship and Ramanujan Fellowship. Dr. Tharamani's research interests include design and development of various carbonaceous materials toward energy conversion and storage, bridging electrochemistry with spectroscopy, and scanning probe techniques, micro-electrochemistry.



Debaprasad Mandal received his Ph.D. in Organometallics Chemistry from the Indian Institute of Technology (IIT) Kanpur, India, in 2006. He joined the Indian Institute of Technology Ropar in 2010 as an Assistant Professor. Prior to join IIT Ropar, Dr. Mandal worked at Erlangen, Germany, as an Alexander von Humboldt fellow for postdoctoral study and then he moved to Texas A&M University as senior scientist. His research work is centered at the interface of organic, organometallics material science, and polymer chemistry. Currently, his group is focused on the development of new ionic liquids, ionic polymers, fluorous materials for catalysis, membrane toward fuel cells, and Li-ion and

Li-S battery. Recently, the group started working on polyoxometalates for electrochemical water oxidation and greener oxidation of organic compound. He is actively involved in research toward energy storage and conversion applications particularly toward advancement of high energy dense batteries by developing highly stable electrolytes and electrode materials.

Aarti Tiwari completed her B.Sc. in Life Sciences (2010) and M.Sc. in Chemistry (2012) from Miranda House, University of Delhi. She later joined the Department of Chemistry, Indian Institute of Technology Ropar in the year 2013 with Dr. Tharamani C. N. Her research interest is toward designing of materials for alkaline fuel cell application followed by in-depth investigation of the processes involved using various physicochemical and electrochemical analysis including the specialized scanning electrochemical microscopy (SECM). She is also involved in the analysis and testing of functionalized electrolytes toward battery applications to enhance the stability and performance of Li-ion cells.

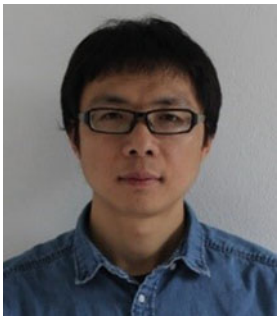
Santosh N. Chavan was born in 1987 and graduated from Balbhim College Beed in 2009. He completed his Master's in Organic Chemistry in the Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad. He has completed his Ph.D. under the guidance of Dr. Debaprasad Mandal in March 2018 in the Department of Chemistry, Indian Institute of Technology Ropar. He received Director Fellowship at IIT Ropar after Ph.D. thesis submission. His major research interest is in ionic liquids and polymers with the applications such as battery electrolytes, non-conventional solvents, lubricants, surface coatings, gas absorption, catalysis, membranes, and electrochemical applications.

Michihisa Koyama received his Ph.D. in Chemical System Engineering from the University of Tokyo in 2002. After serving as Assistant Professor at Tohoku University, he moved to INAMORI Frontier Research Center, Kyushu University, as Professor. He is now serving as Unit Director at the National Institute for Materials Science as well as Professor at Shinshu University and Visiting Professor at Hiroshima University. Dr. Koyama has authored and coauthored more than 270 review articles, books and book chapters, and peer-reviewed journal articles. His research activities cover the wide aspects of energy from materials to systems, further to future energy vision. He was awarded the SCEJ Young Investigator Researcher Award, the Society of Chemical Engineers, Japan, in 2009, and the Young Scientists' Prize, and the Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology in 2014. He directed and participated in more than 60 projects after promotion to Full Professor, which were supported by Japan Science and Technology Agency, Japan Society for the Promotion of Science, New Energy and Industrial Technology Development Organization of Japan, Ministry of the Environment of Japan, leading private companies, etc. He served as committee member of various panels of public organizations for the science policy makings or proposal reviews.

B. Javed received his doctoral degree in the field of Aeronautical and Astronautical Engineering from the University of Tokyo in 2017. He has a multidiscipline research experience in various energy-related technologies, such as thermal-, wave-, and secondary energy devices. He is currently working as postdoctoral fellow in National Institute for Materials Science (NIMS), Japan. His present research focuses on the simulation of the interfacial phenomena for all solid-state Li-ion batteries.

Dajian Li received his Bachelor and Master degrees in Material Science in July 2003 and July 2006, respectively, from Central South University. He obtained his Ph.D. in Material Science from the University of Genoa (Italy) in February 2011. From June 2011, he started his work in KIT as a scientific researcher on the alloy anodes of Li-ion batteries. From May 2017, he started to work on the spinel cathodes on the Li-ion batteries as principal investigator. He is author or coauthor of 25 peer-reviewed publications and a regular speaker in international conferences. His research fields cover experimental and theoretical investigation of phase diagrams. He has been working on lead-free solders, anodes, and cathodes of Li-ion batteries as well as building batteries for various test techniques. He has been awarded for the Highly Cited Research in Intermetallics in December 2016. He was also awarded as recognized reviewer and outstanding reviewer by the Editors of CALPHAD journal.

Weibin Zhang received his Ph.D. in Material Science from Central South University in June 2015. From January to March 2016, he worked as an exchange researcher at the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum. From April 2016 to August 2018, he worked at the Institute for Applied Materials-Applied Materials Physics (IAM-AWP) at Karlsruhe Institute of Technology (KIT) as a scientific researcher. From September 2018, he became a Professor at Shandong University. He is author or coauthor of more than 40 scientific papers in peer-reviewed journals. His research focuses on the integrated computational materials engineering (ICME) and its application for the cemented carbides and Li-ion batteries.



Song-Mao Liang received his Ph.D. from Institute of Metal Research, Chinese Academy of Sciences in 2010. He then worked at the same institute as Assistant Professor. Since July 2017, he works as Research Associate in Clausthal University of Technology. His research interests mainly focus on Calphad modeling and computational thermodynamics applications, such as on light weight alloys, high entropy alloys, Li-ion battery materials and oxides, etc. He has published more than 30 peer-reviewed journal articles and serves as reviewer for more than 10 journals.

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Abbreviations

AC	Activated carbon
AFM	Atomic force microscopy
ASA	Active surface area
^{13}C NMR	Carbon nuclear magnetic resonance spectroscopy
CCCV	Constant current and constant voltage
CCP	Close centered packing
CE	Columbic efficiency
$C_2H_6O_3$	Orthoaceticacid
$C_6H_5CH_3$	Toluene
CID	Current intermitted devices
CMC	Carboxymethyl cellulose
CMD	Chemical manganese dioxide
CPEs	Composite polymer electrolytes
CPR	Current pulse relaxation method
CSTR	Continuous stirred tank reactor
CV	Cyclic voltammetry
DC	Dimethyl carbonate
DFT	Density functional theory
DMSO	Dimethyl sulfoxide
DOD	Depth of discharge
DOT	US Department of Transportation
dQ/dE	Differential capacities
DSC	Differential scanning calorimetry
EC	Ethylene carbonate
EDS	Energy dispersive X-ray spectroscopy
EELS	Electron energy loss spectroscopy
EIS	Electrochemical impedance spectroscopy
EO/PO	Ethylene oxide/propylene oxide
EPDM	Ethylene-propylene-diene methylene
FTIR	Fourier transform infrared spectroscopy
GIC	Graphite intercalation compounds
GO	Graphene oxide
GPC	Gel permeation chromatography

^{1}H NMR	Proton nuclear magnetic resonance spectroscopy
HAADF	High-angle annular dark-field
HCP	Hexagonal close-packing
HEV	Hybrid electric vehicle
HF	Hydrogen fluoride
HFP	Hexafluoropropylene
HOMO	Highest occupied molecular orbital
HOPG	Highly oriented pyrolytic graphite
HR-TEM	High-resolution transition electron microscope
IC	Ion chromatography
IL	Ionic liquid
ITO	Indium tin oxide
LAGP	Lithium aluminum germanium phosphate
LATP	Lithium aluminum titanium phosphate
LCO	Lithium cobalt oxide
LFP	Lithium ferrophosphate
LGPS	Lithium germanium phosphorous sulfide
Li	Lithium
Li^+	Lithium ion
Li_2CO_3	Lithium carbonate
Li_3PO_4	Lithium phosphate
$LiAlO_2$	Lithium aluminate
LiBOB	Lithium bis(oxalato) borate
LIBs	Lithium ion batteries
$LiClO_4$	Lithium perchlorate
$LiPF_6$	Lithium hexafluorophosphate
LiPON	Lithium phosphorus oxynitride
LiTFSI	Lithium bis(trifluoromethylsulfonyl)imide
LLTO	Lithium lanthanum titania
LLZO	Lithium Lanthanum zirconia
LMO	Lithium manganese oxide
LPS	Lithium phosphorous sulfur
LSM	Layer-structured material
LTN	Li-ion transference number
LTO	Lithium titanate
LUMO	Lowest unoccupied molecular orbital
LZP	Lithium zirconium phosphate
MCF	Graphitized mesophase carbon fiber
MCI	Mixed conducting interphase
MEC	Methyl-ethyl carbonate
MO	Molecular orbital
NCA	Lithium nickel cobalt aluminum oxide
NCM	Lithium nickel cobalt manganese oxide
NF	Nanofiber