2022

Second Quarter

PTC Newsletter

PTC Polymer Technology Consortia

UPCOMING EVENTS

Mark Your Calendars for the PTC Fall meetings!

Scratch Behavior of Polymers Consortium-SCRATCH

SCRATCH FALL meeting-October 13^{h}, 2022
Texas A&M University-College Station, TX

Polymer Technology Industrial Consortium-PTIC

PTIC FALL meeting—October 13^{th}-14^{st}, 2022
Texas A&M University-College Station, TX

Inside the Newsletter

"Polymer passivation films for lithium metal electrodes"

Perla Balbuena, Chemical Engineering

Perla B. Balbuena is Professor, and Mike O'Connor Chair I in the Artie McFerrin Department of Chemical Engineering at Texas A&M University. She holds joint (courtesy) appointments in the Department of Chemistry and Department of Materials Science and Engineering. Her research group focuses on first-principles computational analysis and design of materials properties and processes, with main applications to catalysis, electrocatalysis, and battery materials. A large component of Dr. Balbuena's work centers on interfacial processes, which are crucial in a variety of problems ranging from reactions on catalytic surfaces, to transport/chemistry in biological membranes, and to battery lifetime links to charge and discharge events. Balbuena's group uses the most advanced atomistic-based simulation techniques to elucidate microscopic-scale events that define macroscopic behavior. Over the years, Balbuena's research has received support from NSF (including CAREER and POWRE Awards), ARO, DOE Basic Energy Sciences, ARPA-E, and DOE-EERE, for her work in these areas. In the past 20 years, Prof. Balbuena's group has contributed to developing a thorough understanding of microscopic processes relevant to the development of longer life, higher density advanced batteries. In this sense, one of the crucial aspects behind battery degradation processes, is the development of a passivation layer at the electrode surfaces during battery cycling. Because the passivation behavior depends crucially on the electrolyte, significant experimental and theoretical work is dedicated to understanding electron and ion transport at these interfaces. Dacheng Kuai, a chemistry PhD graduate student in Balbuena's group, has contributed to the elucidation of polymerization reaction mechanisms in electrochemical interfaces. His work, recently published in *ACS Applied Materials and Interfaces* (https://doi.org/10.1021/acsami.1c20487), identifies the mechanisms for initiation, growth and termination of a polymer film due to electrolyte degradation at the electrode surface.

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Kuai and Balbuena's results identified the most kinetically favored pathways for polymerization of ethyl and vinyl carbonates (EC and VC). The findings highlight differences in the initiation reactions, with VC ring-opening initiation and early-stage propagation more favorable than the corresponding EC processes, while poly(VC) formation has the smallest barriers among all the proposed self-polymerization pathways. Cross couplings between the VC molecule and EC radicals were also characterized. Barriers for these processes were also considerably smaller than EC self-polymerization. Therefore, inclusion of VC additive significantly reduces the energy cost for EC chain propagation. In current work, in collaboration with Prof. Ulrike Krewer's group from Karlsruhe Institute of Technology (Germany), these calculated energetic barriers and the details of the polymerization pathways are input to a coarse-grained Kinetic Monte Carlo model that will allow us to follow the polymerization process in real time, and simultaneously with other surface passivation reactions.

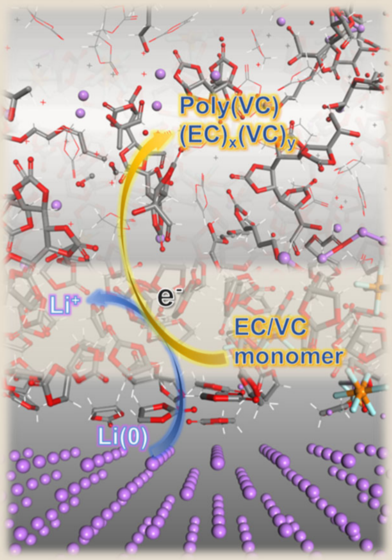


Figure 1. Electron-induced electrolyte solvent polymerization near lithium metal anode surface.

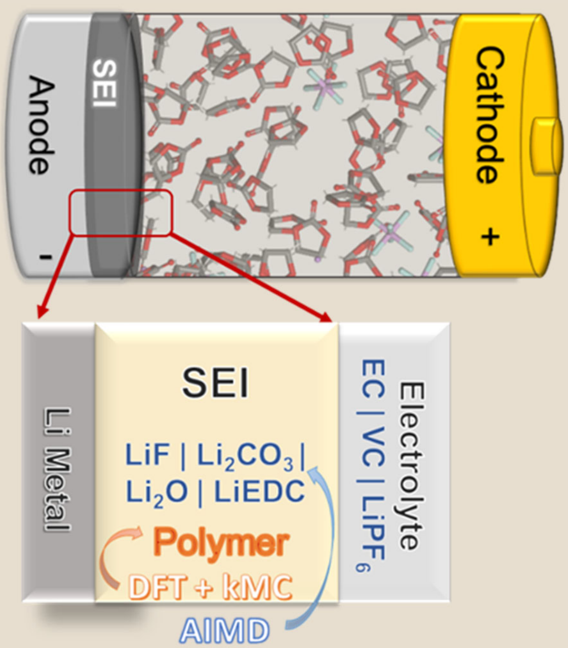
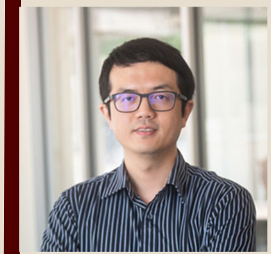


Figure 2. First principle simulation of the lithium metal battery SEI formation at metal-liquid interface.



"Climbing the ladder to advanced applications of ladder polymers"

Dr. Lei Fang, Chemistry Department

Dr Lei Fang is an Associate Professor in the Department of Chemistry at Texas A&M University. He began his PhD study at University of California Los Angeles, and received the degree at Northwestern University in 2010, mentored by Professor Sir Fraser Stoddart. Subsequently, he spent two and a half years at Stanford University as a postdoctoral scholar working with Professor Zhenan Bao. AT TAMU, Dr Fang's research interests spans a broad range of fields on chemical innovation for functional organic materials, with focuses on conjugated ladder polymers, rigid organic pi-systems, porous polymer networks, organic/inorganic composite materials, and supramolecular chemistry. His research involves fundamental scientific investigations on chemical synthesis, physical organic chemistry, polymer physics, and materials science, *etc*.; as well as application developments on organic electronics, clean energy, separation, smart materials, catalysis, and industrial innovation, *etc*. Dr Fang's achievements on research and education have been recognized by a number of awards and honors, including the Kaneka Junior Faculty Award (2015), NSF CAREER Award (2017), Montague Center for Teaching Excellence Scholarship (2017), *Polymers* Young Investigator Award (2018), the Texas A&M University Presidential Impact Fellowship (2020), and the Humboldt Research Fellowship for Experience Researchers (2022). Lei Fang has published over 90 peer-reviewed publications and given >70 invited lectures.

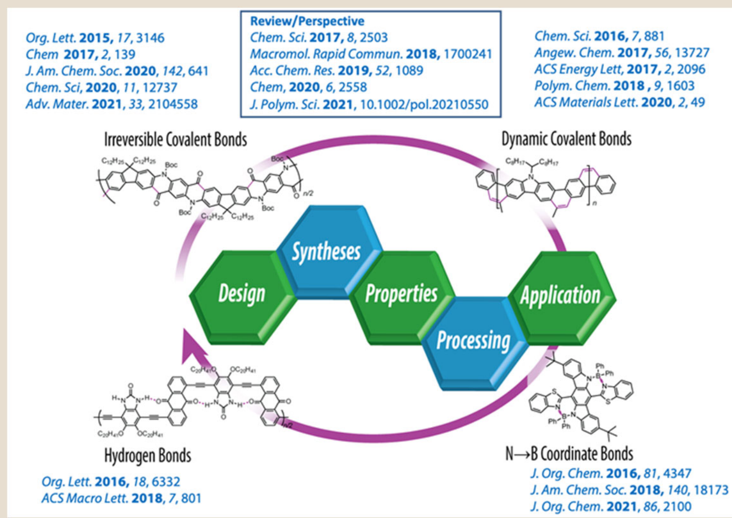


Figure 1. Summary of Lei Fang's work on conjugated ladder polymer chemistry.

Dr Fang's group represents one of the world leading teams in the field of conjugated ladder polymers. A conjugated ladder polymer features more than one strands of bonds connecting the conjugated macromolecular backbone, so that they are intrinsically distinctive compared to well-studied conventional single-stranded polymers. The chemical synthesis, characterization, and polymer physics of ladder polymers are highly intriguing and significant in terms of advancing fundamental polymer science. In addition, conjugated ladder polymers are promising on account of their unconventional yet favorable electronic and mechanical properties that are inaccessible in conventional single-stranded polymers. However, research on these polymers are formidably challenging due to the need of constructing multiple strands of bonds during synthesis, and the elusive polymer physics associated with the rigid backbone. Throughout his independent research career, Dr Fang's team has made significant, deep, and broad contributions to this challenging and unconventional research field (**Figure 1**).

Continue on next page

Continue from page 2—"Climbing the ladder to advanced applications of ladder polymers"

Dr Fang's accomplishments on the syntheses of ladder polymers and fused-ring small molecules provided new foundations for the development of novel stimuli responsive materials and functional porous materials. Including stimuli responsive materials and functional porous materials.

By compositing a ladder polymer with carbon nanotube sheets in a bilayer configuration, Dr Fang's team achieved the fabrication of a high-performance, extraordinarily robust jumping actuator (**Figure 2**). The unprecedented performance and stability of this composite originated from the unique chemical constitution of the conjugated ladder polymer backbone, leading to their great promises for future applications in soft robotics. In a separate project, they developed a feasible strategy to fabricate thermal fluorescent polymer composite, by manipulating the supramolecular aggregation and dissociation of ladder-type quinacridone molecules in micrometer-sized solution capsules in a polymer matrix. This composite material shows high contrast, turned-on fluorescence upon heating, excellent reversibility due to the supramolecular nature of the thermofluorescence mechanism, and feasible tunability of the thermal transition temperature.

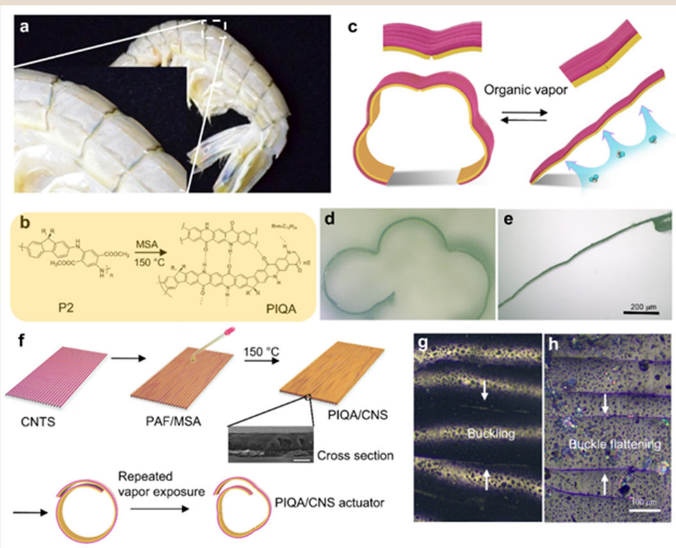


Figure 2. Graphical illustration of shrimp-like jumping actuator composed of conjugated ladder polymer and carbon nanotube sheet.

The low entropy nature of ladder polymer attracted Dr Fang's attention for gas adsorption applications, based on the hypothesis that a porous ladder polymer network would suffer a much smaller entropy penalty upon gas adsorption due to its lower initial entropy (**Figure 3**). The team tested and validated this hypothesis on a model porous ladder polymer network. A significantly lower adsorption entropy cost for the ladder polymer networks was noted, accompanied by an ultra-high gas uptake capacity per unit surface area. These findings here constitute an important orthogonal strategy to increase the gas adsorption capacity of porous materials and to improve their high temperature performances, which are critical for clean energy applications. In addition, Dr Fang's team established an aldol-triple condensation method to synthesize porous materials. Preorganized porous graphitic carbon was successfully synthesized from a specifically designed monomer. The material shows high microporosity and narrow pore size distribution at ~0.6 nm. More interesting, it demonstrates high tendency of graphitization originated from the preorganized aromatic framework in the network, allowing for a graphitization temperature significantly lower than those required on conventional graphite precursors. This exciting development is highly promising for the development of next generation electrocatalyst on account of the tolerance of functional catalytic components in the porous graphitic carbon by avoiding high heat.

Dr. Lei Fang Continue —"Climbing the ladder to advanced applications of ladder polymers"

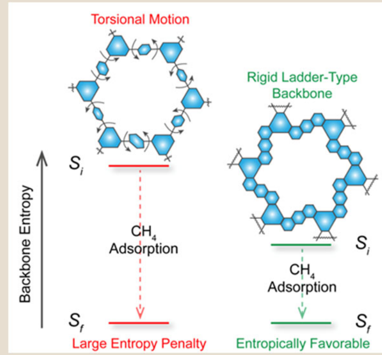


Figure 3. Low entropy penalty in gas adsorption promoted by rigid ladder-type backbone of a porous material.

Online engineering program again ranked No. 1 in Texas

Texas A&M University's College of Engineering was again ranked No. 1 in the state of Texas for its online graduate engineering programs.

The latest ranking, from U.S. News and World Report's 2022 Best Online Programs, rates Texas A&M's online master's engineering program ninth in the nation, tied with the Missouri University of Science and Technology and the University of Wisconsin-Madison.

Full story: **https://bit.ly/3NRvpBU**

Engineering faculty named National Academy of Inventors Senior Members

The three new senior members from the College of Engineering are:

Dr. Melissa Grunlan, Charles H. and Bettye Barclay Professor in Engineering in the Department of Biomedical Engineering.
Dr. Andreas Polycarpou, James J. Cain Chair in the J. Mike Walker '66 Department of Mechanical Engineering.
Dr. Taylor Ware, associate professor in the Departments of Biomedical Engineering and Materials Science and Engineering.

NAI Senior Members are active faculty, scientists and administrators from NAI member institutions who have demonstrated remarkable innovation-producing technologies that have brought, or aspire to bring, real impact on the welfare of society. They also have growing success in patents, licensing and commercialization, while educating and mentoring the next generation of inventors.

Full story: **https://bit.ly/3jjenP7**

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Dr. Hong-Mao Wu
PTC Visiting Scholar—Taiwan

Dr. Hong-Mao Wu finished his visiting scholar project in Dr. Sue's lab in January of 2022. His research focused on the structure-properties relationship of the multi-functionalities polymer nanocomposite. The research project was funded by a Kaneka Visiting Scholarship in 2020. I developed several novel inorganic/polymer nanocomposite systems and filed two patents in these two years. I really enjoyed working with Dr. Sue's Group, not only in research but also in extracurricular activities. Even under the epidemic, I had an unforgettable two-year life as a visiting scholar at TAMU.

Dr. Yen-Ting Lin
PTC Visiting Scholar—Taiwan

Dr. Yen-Ting Lin really appreciated the efforts made to allow him to participate in the Visiting Scholar Program at TAMU during which he worked with Professor Hung-Jue Sue.

During the visit Yen-Ting was introduced to new ways of doing research and the diverse experience seems to be rewarding like as research has constantly demonstrated that it helped to update knowledge, improve research capabilities and problem-solving skills, enrich cross-cultural collaboration, increase joint research program. Yen-Ting felt especially fortunate that he was able to hear from a series of speakers who addressed a central question about the latest research and development projects related to polymers, those significant experience and great interacted lessons are available to enrich every step of his career for the future.

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Polymer Specialty Certificate Updates

Students that have applied for the Polymer Specialty Certificate	87
Students that have received the Polymer Specialty Certificate	75

For more information, please visit: http://ptc.tamu.edu/polymer-specialty-certificate/

Have Questions?

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