2022
Third Quarter
PTC Newsletter

PTC Polymer Technology Consortia

UPCOMING EVENTS

Mark Your Calendars for the PTC Fall meetings!

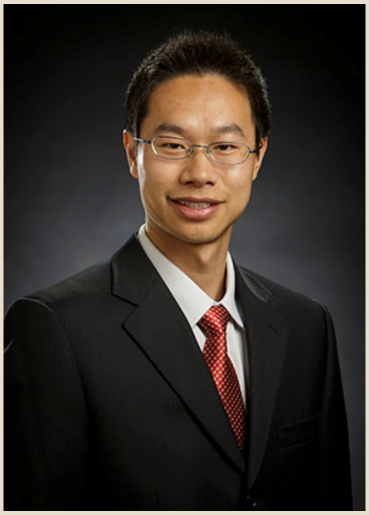
Scratch Behavior of Polymers Consortium-SCRATCH

SCRATCH FALL meeting-October 13th, 2022
Texas A&M University-College Station, TX

Polymer Technology Industrial Consortium-PTIC

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

Inside the Newsletter



"Engineering Metal-Organic Framework-Based Polymer Composites for Industrial Applications"

Qingsheng Wang, Chemical Engineering

Dr. Qingsheng Wang is an Associate Professor of Chemical Engineering and George Armistead '23 Faculty Fellow at Texas A&M University. He was Dale F. Janes Endowed Professor and Department Head of Fire Protection & Safety at Oklahoma State University before his return to TAMU in 2019. Dr. Wang received his BS and MS degrees in Chemistry with Honors and PhD degree in Chemical Engineering at TAMU, mentored by Professor M. Sam Mannan (Chemical Engineering) and Professor F. Albert Cotton (Chemistry). He has nearly 15 years of work and research experience in the areas of chemical engineering, chemistry, and materials science and engineering. Dr. Wang has published over 150 peer-reviewed journal publications, 6 book chapters, and 2 patents pending. His work has been internationally recognized and heavily cited, and he is recognized as the world leader in process safety area. He is the Subject Editor for *Process Safety and Environmental Protection* (Elsevier) and Associate Editor for *Journal of Thermal Analysis and Calorimetry* (Springer). He is a principal member of NFPA 18 and 30 committees. Dr. Wang is a egistered professional engineer and certified safety professional. He has provided professional consulting for chemical, petrochemical, and oil & gas industries. Dr. Wang is currently leading an active research group, pioneered in the areas of flame-retardant polymers, fire & explosion dynamics, and smart materials for safety and sustainability.

The polymeric materials provide numerous advantages to society in everyday life. However, there is a continuous demand for improved properties of polymeric materials especially when they are extended for use in new applications with increasingly stringent requirements. Metal–organic frameworks (MOFs) are a class of

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crystalline materials with permanent porosity, having wide applications including gas purification, gas separation, water remediation, catalysis, energy storage, and drug delivery. Due to their inorganic–organic hybrid nature, MOFs have greater compatibilities with polymers to form composites. Dr. Wang's group has contributed to developing MOF-polymer composites and improving their properties for increasingly stringent requirements.

Among the properties of polymers, the low propensity of ignition and/or improved flame retardancy is of great importance, given the fact that polymeric materials are taking an increasingly large portion of the fire load in houses, commercial environments, and transportation. In this sense, Ruiqing Shen et al. have contributed to using metal–organic framework (MOF) as an efficient synergist for intumescent flame retardants (IFR) against highly flammable polypropylene. Our work has recently been published in *Industrial & Engineering Chemistry Research* (https://doi.org/10.1021/acs.iecr.2c00715). In this study, zeolite imidazolate frameworks-8 (ZIF-8), a commercially available MOF from BASF, was incorporated into an IFR/polypropylene (IFR/PP) composite system. The results show that ZIF-8 and the IFR additives exhibit a strong synergistic effect between them for improvement of the formation and stability of the intumescent char layer, to prevent the intensive burning of PP. As shown in Figure 1, by adding only 2 wt % of ZIF-8, its limiting oxygen index value reached 31.2% and it obtained a UL-94 V-0 rating. Furthermore, the addition of ZIF-8 could contribute to reducing the burning intensity and suppressing the smoke release as well as CO and CO_2 production from burning IFR/PP composites. This study provides new insights for developing more efficient IFR systems for polyolefins and reducing their smoke emissions during combustion. Since all the raw materials are commercially available and the preparation method is compatible with current industrial processes, the methodology presented in this study is ready for industrial application.

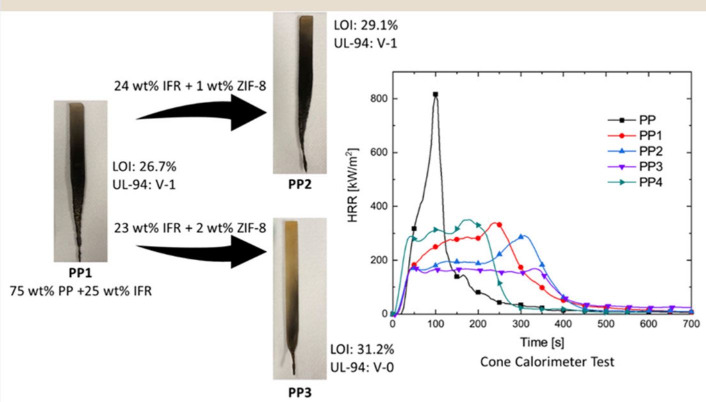


Figure 1. Metal–organic framework (MOF) as an efficient synergist for intumescent flame retardants (IFR) against highly flammable polypropylene.

Currently, most MOF-polymer composites are prepared by a discretely bottom-up principle, where different MOFs are firstly synthesized through complex hydrothermal reactions and further blended within different polymers in solutions, such as mixed-matrix membranes (MMMs) and polymer-grafted MOFs. As illustrated in Figure 2, such processes include several sophisticated deposition methods onto the matrix, thus requiring tedious time, solvent, and energy. This is very challenging for efficiently and sustainably manufacturing of MOF-polymer composites on an industrial scale. Therefore, with the aim of advancing the scalable applications of MOFs and improving the properties of polymer matrix, our recent published paper by Yufeng Quan et. al in *ACS Sustainable Chemistry & Engineering* (https://doi.org/10.1021/acssuschemeng.2c01720) proposed that the MOF synthesis and subsequent composite blending could be combined into one sustainable and efficient step via reactive extrusion. Compared with the conventional hydrothermal synthesis route, we can efficiently achieve production capacity from ~30 g/day (1 L batch reactor) to ~10 kg/day (Process 11 parallel twin-screw extruder) MOF-polymer nanocomposites. To investigate the feasibility of this one-step reactive extrusion method, two types of widely used polymer matrix, polypropylene (PP) and polystyrene (PS), are chosen to manufacture different pressed-stable MOF nanocomposites. Zeolitic imidazolate frameworks (ZIFs), specifically ZIF-8 and ZIF-67 are chosen as example MOFs for this process. The improvements on the thermal stability, flammability, and mechanical properties of the polymer matrix are also discussed, as well as their applications as catalysts in wastewater contaminants degradation. Compared with the conventional solvothermal method, notable throughput rate and space time yield explored in this work provide an efficient and sustainable area for potentially scaling up MOF-polymer applications in industry via a combination of the reaction and blending steps.

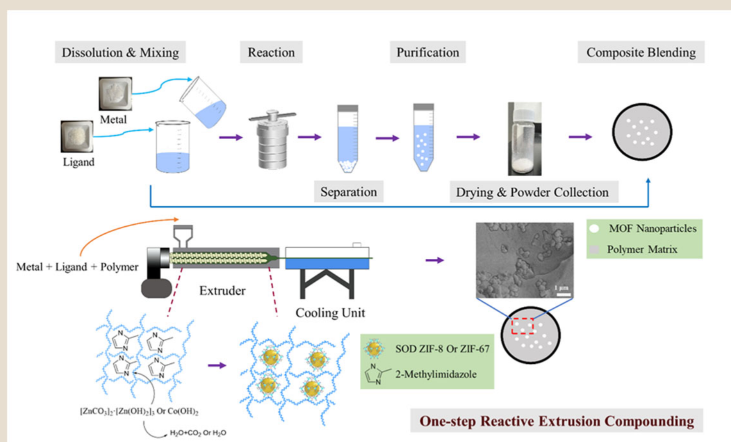
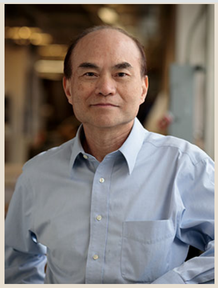


Figure 2. Schematic illustration on the one-step reactive extrusion compounding method for MOF-polymer nanocomposites manufacture

"Polypropylene with improved electrical and thermal conductivity"



Hung-Jue Sue
Materials Science and Engineering

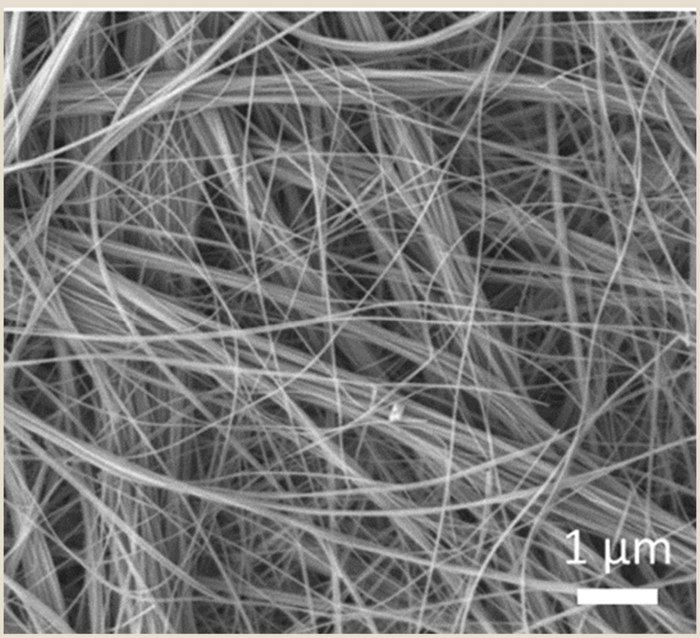
Polypropylene is a commodity thermoplastic with many useful properties. For some applications such as electrical housings and electronic packaging, improved electrical and thermal conductivity would be desirable to reduce EMI (electromagnetic interference) and heat transfer for better cooling.

We've been working on using copper nanowire (CuNW) as additives for thermoplastics. For CuNW to be effective, it must be dispersed without significant aggregation, which would require increased loadings for a given level of conductivity. Another difficulty to overcome is oxidation during preparation and blending, which reduces the inherent conductivity of copper metal. This is a challenge because of the high ratio of surface to volume in these small-diameter (~20 nm) wires.

The CuNW is prepared by adding a reducing agent (glucose) to an aqueous solution of copper chloride. An amine (hexadecylamine) is also added which serves two roles. It promotes the formation of nanowires rather than a more conventional morphology with lower aspect ratio. It also forms a monolayer on the CuNW surface, greatly reducing the rate of oxidation.

When the CuNW is mixed with polypropylene using a solution process at a 2.5 wt% loading, the electrical conductivity jumps to 500 S/cm, an increase of 16 orders of magnitude. The thermal conductivity increased by 234%.

We are continuing to work on CuNW as an additive to polymeric materials. This on-going project is being done in collaboration with the Formosa Plastics Corporation.



As-produced copper nanowire (CuNW)

Pentzer selected as finalist for 2022 Blavatnik National Award

The New York Academy of Sciences and the Blavatnik Family Foundation named Dr. Emily Pentzer a finalist for the 2022 Blavatnik National Award for Young Scientists in Physical Sciences & Engineering, which honors the achievements and potential of rising researchers.

Moving forward, she hopes to use this accomplishment as a catalyst to support the various research ventures her group is pursuing.

The Blavatnik National Awards will be presented at the American Museum of Natural History in New York City on Tuesday, September 19.

Full story: **https://bit.ly/3t8cXMr**

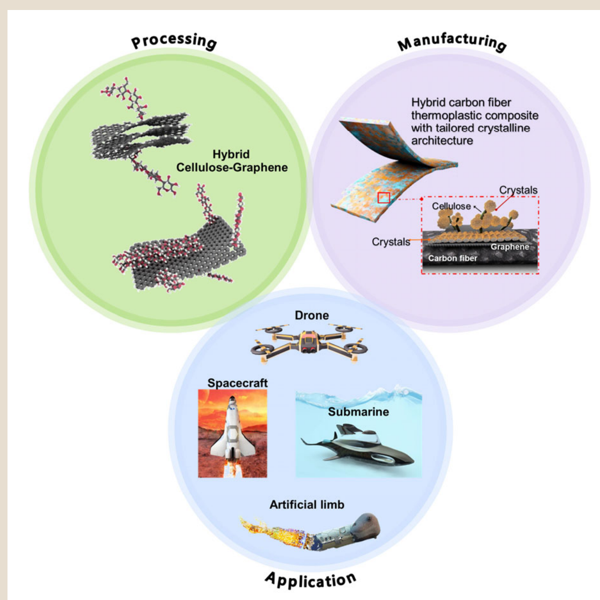
New method for thermoplastic production offers potential to replace metals

Amir Asadi, Engineering Technology & Industrial Distribution

Funded by the National Science Foundation's (NSF) Faculty Early Career Development (CAREER) Award, Dr. Amir Asadi, assistant professor in the Department of Engineering Technology and Industrial Distribution at Texas A&M University, has developed a method using hybrid nanomaterials capable of creating high-performance thermoplastic composites with favorable mechanical properties within minutes.

Fiber-reinforced thermoplastics are replacing metals at high rates because of their inherent properties — they are light, strong, recyclable and malleable. They can be used in various applications including manufacturing, automobile and aerospace industries, because they are both cost-effective and sustainable.

Full story: **https://bit.ly/3MGE7Id**



Fiber-reinforced thermoplastics can be used in various applications including manufacturing, automobile and aerospace industries, because they are both cost-effective and sustainable.

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On April 22nd, 2022 at the Polymer Technology Industrial Consortium meeting the following scholarship recipients were recognized.

L-R: Jose Guerrero, AERO; **Donna Davis, SPE Liaison** and Hailey Young, INEN. Congratulations to these undergraduates students for being the recipients of the SPE Dale Walker Memorial scholarship.

L-R: Kartik Rajagopalan, MSEN; **Dr. David Hansen, SPE Liaison** and Zewen Zhu, MSEN. Congratulations to these graduate students for being the recipients of the SPE Henry Kahn Memorial scholarship.

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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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PTC Polymer Technology Consortia
Materials Science & Engineering

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