# Fast-Tracking Next-Gen Polymers: How SABIC is Leveraging Machine Learning and Physics

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Polymeric materials touch almost every facet of our daily lives, ranging from automobiles to energy storage to electronics to paints and coatings. Polymers are widely utilized because they are affordable, light weight, flexible, and easy to manufacture. However, despite significant advances in performance of polymeric materials over the past decades, designing new polymers that have enhanced properties, such as better stability, optical properties or biodegradability, remains a critical challenge. While there are boundless possibilities to modify the underlying chemical structure when designing new plastics, the classic approach typically relies heavily on trial-and-error experimentation that is slow and expensive. Adding to the complexity, when researchers improve one aspect of the plastic, it often makes another aspect worse. Designing new polymer materials is like solving a complicated puzzle which requires optimizing multiple properties simultaneously, also known as multiparameter optimization (or MPO).

To efficiently identify new polymers for optical applications with improved properties and reduce the reliance on expensive trial-and-error experimentation, Saudi Basic Industries Corporation (SABIC)'s Specialties business is leveraging Schrödinger's computational platform for polymer modeling and materials informatics. The resin design and incubation team at SABIC worked closely with Schrödinger's material science team to build accurate machine learning (ML) models to speed up the discovery of new polymers. "The computationally driven approach we have employed has demonstrated strong potential to accelerate the design and discovery of new polymers for our targeted applications, such as in mobility, infrastructure, 5G, medical devices, coatings and more," says André van Zyl from SABIC.

One of the key challenges in materials science is the availability of reliable data, which can be used to train the ML models to accurately explore targeted polymer properties. SABIC has curated an extensive experimental dataset consisting of five target properties related to how polymers respond to temperature changes, electrical exposure, mechanical stress, and optical conditions. The team successfully trained and validated ML models that accurately predict the five polymer properties. "These ML models are advantageous because they are predictive of polymer properties using only the molecular structure as input, which means we can use these models to rapidly identify polymers that strike a balance between the five key properties," says Alex Chew from Schrödinger.

Schrödinger and SABIC then used the trained ML models to explore new polymer structures that have not yet been tested

experimentally and that exhibit polymer properties useful to real-world applications. The team generated a large library of over 10,000 structures, deployed the trained ML models to predict the polymer properties across the enumerated structures, and applied a MPO ranking criteria to identify structures with preferred polymer characteristics. With Schrödinger's collaborative enterprise informatics platform, LiveDesign, the team narrowed down the design space to 1,000 structures by accounting for the desired preference of each polymer property. From these 1,000 structures, the team pinpointed commercially available structures, which were then narrowed to ten experimentally viable structures with promising properties.

> "With the success of this project, we are now inspired in adopting a 'computation-first' approach in our current and future projects."

"To give us further confidence in these ten candidate structures, we tested using physics-based approaches, and the outcomes were consistent with those predicted by in ML models. Employing a combined data-driven and physics-based approach helps lower the chances of failure in experiments," says Atif Afzal from Schrödinger.

"We experimentally evaluated three of the ten candidate structures, and they satisfied all the criteria we initially set out to achieve. These computational results are highly promising and can potentially shorten our polymer innovation timelines from traditionally a couple of years to only a couple of months.," said Vaidya Ramakrishnan from SABIC.

Not only has this computationally driven workflow sped up the innovation of new polymers, but it has also inspired scientists to leverage computational tools to test significantly more novel structures that would not have been feasible through trial-and-error experimentation alone.

## Vaidya Ramakrishnan, Ph.D.

Dr. Vaidya Ramakrishnan is a Staff Scientist with SABIC's specialty business with a research background in polymer physics and polymeric materials design. Vaidya joined GE-Plastics in 2005 and continued with SABIC from 2007 and has a PhD in Mechanical Engineering (Polymer Technology) from Technical University-Eindhoven.

## André van Zyl, Ph.D.

Dr. André van Zyl earned his Ph.D. in Polymer Science from the University of Stellenbosch in 2003. He has been involved in product development since 2006 when he joined GE Plastics in Bergen op Zoom (The Netherlands) and has since then journeyed onwards to SABIC in 2007 leading various materials platforms including amorphous, semicrystalline as well as thermoplastic composite materials.

## Alex K. Chew, Ph.D.

Dr. Alex K. Chew is a Senior Scientist at Schrödinger passionate about integrating physics-based tools and machine learning to accelerate materials design. Alex earned his B.S./M.S. from NYU Tandon School of Engineering in 2016, followed by his Ph.D. in Chemical Engineering from the University of Wisconsin-Madison in 2021.

## Atif Afzal, Ph.D.

Dr. Atif Afzal is a Principal Scientist at Schrödinger, working in the Material Science division to improve molecular simulation tools and provide scientific solutions to industrial partners. Atif pursued his undergraduate education at the Indian Institute of Technology Kanpur and completed his doctoral studies in Chemical Engineering at the University at Buffalo.

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