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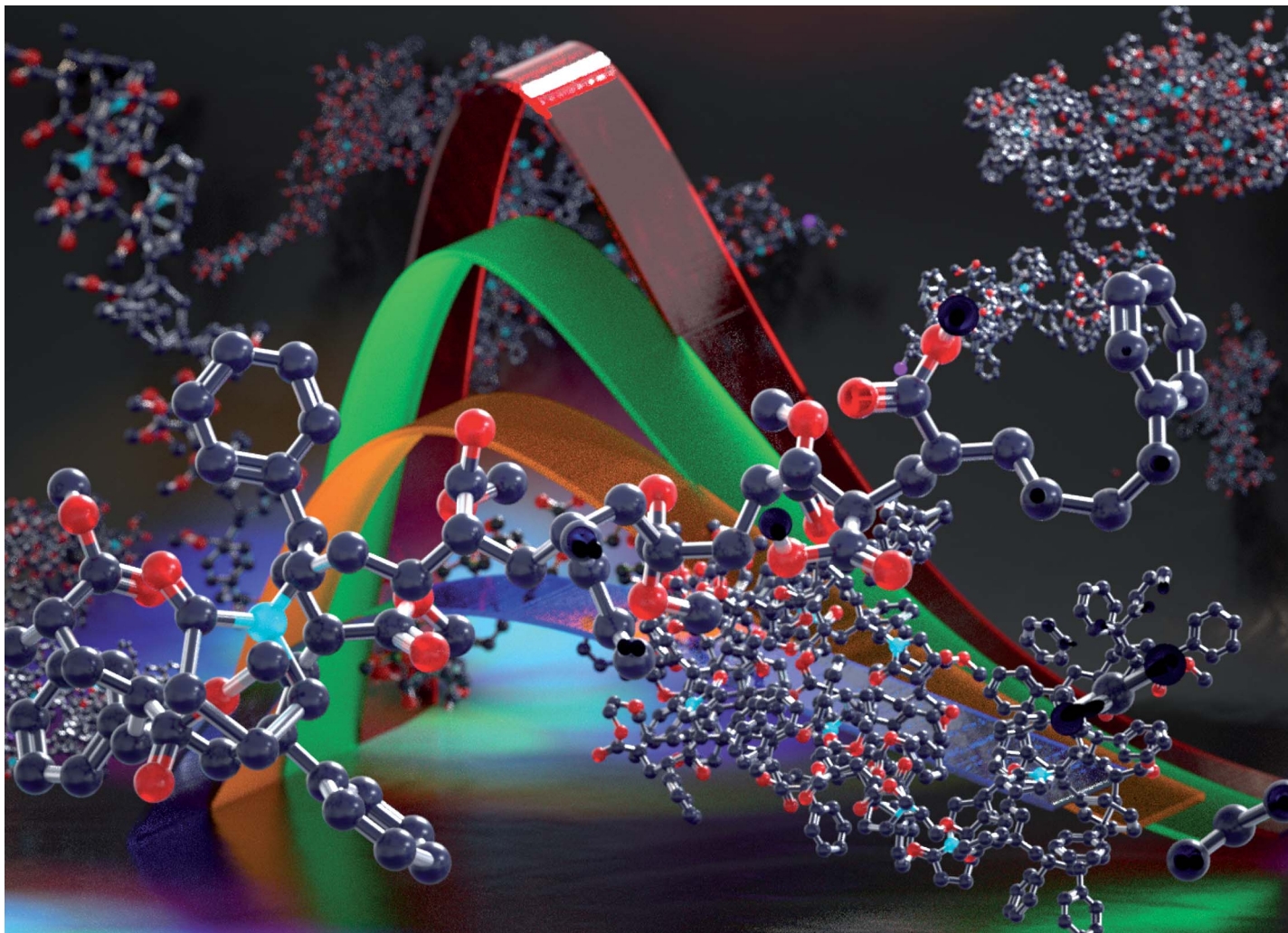
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Showcasing research from Professor de Pablo's laboratory,  
University of Chicago, IL, USA.

Generative BigSMILES: an extension for polymer  
informatics, computer simulations & ML/AI

Generative BigSMILES (G-BigSMILES) enhances the  
BigSMILES line notation for representing polymer ensembles.  
It includes reactivity ratios, molecular weight distributions,  
and ensemble size data to facilitate molecule generation. This  
notation streamlines AI-driven accelerated materials design  
and advancements in polymer science. The code for this  
research can be found at [https://github.com/InnocentBug/  
bigSMILESgen](https://github.com/InnocentBug/bigSMILESgen).

As featured in:



See Ludwig Schneider,  
Juan de Pablo *et al.*,  
*Digital Discovery*, 2024, 3, 51.