Teaching an old dog a new trick: polymer mechanochemistry of triarylmethanes

Dr. José Augusto Berrocal
Research ICIQ

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Teaching an old dog a new trick: polymer mechanochemistry of triarylmethanes

José Augusto Berrocal
Institute of Chemical Research of Catalonia (ICIQ), Avda. Països Catalans 16, 43007 Tarragona, Spain

Polymer mechanochemistry studies the interaction between mechanical force and polymer materials in fluid- and solid-state systems by developing so-called mechanophores.[1] The latter are chemical motifs that generate physicochemical signals in response to the force-induced cleavage of intentionally labile bonds (Figure 1a).[1] Some mechanophores exhibit the particularly attractive feature of being mechanochromic, meaning that they change their optical properties (absorption or emission of light) as a consequence of the bond cleavage event.[2] This has paved the way for their use as force sensors to predict/anticipate the end-of-life or catastrophic failure of polymer materials with molecular resolution. Other recent applications of judiciously designed mechanoreponsive designs include unmasking latent functionalities such as catalysis, acidity, and small molecule/drug release.[2]

In this talk, I will discuss our latest developments on heterolytic mechanophores, *i.e.*, motifs that dissociate into ion pairs upon mechanical stimulation, based on the triarylmethane skeleton (**Tr**, Figure 1b). **Tr** species have already been shown to dissociate into brightly colored, resonance-stabilized triarylcarbenium ions ($\mathbf{Tr}^+$, Figure 1b) and anionic counterparts (Figure 1b, X = OH, CN, …) by treatment with acids or irradiation with light.[3] Our group has recently demonstrated that a similar transformation can also be triggered by mechanical stimulation of solid-state polymers comprising **Tr** species.[4] The process can be followed by performing uniaxial deformation experiments in conjunction with optical techniques in a home-built setup.[4] The color and nature of the mechanochromic response can be tuned via simple structural modifications.[5] Further research developments from our group will also be discussed.

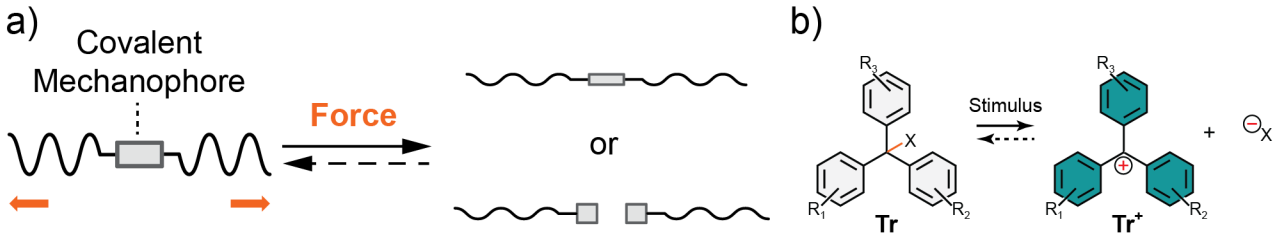

Figure 1. (a) Schematic representation of force-triggered reactions of covalent mechanophores. (b) Stimulus-induced heterolytic dissociation of triarylmethane derivatives (**Tr**) into triarylcarbenium ions ($\mathbf{Tr}^+$) and anionic counterparts (X^-).

References

(1) Li, J.; Nagamani, C.; Moore, J. S. Polymer Mechanochemistry: From Destructive to Productive. *Acc. Chem. Res.* **2015**, *48* (8), 2181–2190.
(2) Abi Ghanem, M.; Basu, A.; Behrou, R.; Boechler, N.; Boydston, A. J.; Craig, S. L.; Lin, Y.; Lynde, B. E.; Nelson, A.; Shen, H.; Storti, D. W. The Role of Polymer Mechanochemistry in Responsive Materials and Additive Manufacturing. *Nat. Rev. Mater.* **2021**, *6*, 84–98.
(3) Gessner, T.; Mayer, U. Triarylmethane and Diarylmethane Dyes. *Ullmann's Encycl. Ind. Chem.* **2012**, *37*, 425–478.
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(5) Hemmer, J.; Bauernfeind, V.; Rader, C.; Petroselli, M.; Weder, C.; Berrocal, J. A. Triarylmethane Mechanophores Enable Full-Visible Spectrum Mechanochromism. *Macromolecules* **2023**, *56*, 8614–8622.

Biography

https://iciq.org/staff/berrocal-jose/

Dr. José Augusto Berrocal was born in Orvieto, Italy, in 1986. He obtained his Ph.D. in Chemistry (2014) from the University of Rome "La Sapienza". During his doctoral studies, he was trained as a physical organic chemist under the guidance of Prof. Luigi Mandolini and Prof. Stefano Di Stefano.

In 2014, Dr. Berrocal relocated to the Netherlands as a postdoctoral fellow at Eindhoven University of Technology, working with Prof. E.W. "Bert" Meijer. Three years later, he joined the group of Prof. Ben Feringa at the University of Groningen. These experiences provided him expertise in supramolecular chemistry and materials, and light-driven molecules and molecular systems.

Dr. Berrocal embarked on his independent career at the Adolphe Merkle Institute (AMI) of the University of Fribourg (Switzerland) in September 2019. In his independent research, he started combining concepts and techniques from organic, supramolecular, and polymer chemistries to tackle scientific challenges that exceed one specific field of interest. Designing and understanding stimuli-responsive materials devoted to potential sustainable and environmental applications constitutes a major drive in his research.

In July 2023, Dr. Berrocal assumed the role of Group Leader at ICIQ as part of ICIQ's Starting Career Programme (ICIQ-SCP) funded by the Severo Ochoa Excellence Grant CEX2019-000925-S (MCIN/AEI/ 10.13039/ 501100011033). He has started this new phase also with an ERC Starting Grant for the project "Reversible Heterolytic Mechanophores for Dynamic Bulk Materials" (ReHuse).

Dr. Berrocal has been recognized with the 2023 Thieme Chemistry Journals Award and the 2024 Outstanding Young Researcher in Polymers from the Group Specialized in Polymers (GEP) of the Royal Spanish Chemical Society (RSEQ). He has been serving as an Editorial Advisory Board Member for ACS Macro Letters since January 2024.