Stress causes molecules to change color

You may have heard of mood rings that change color depending on the wearer's mood (caused by changes in temperature); but have you heard about films that change color upon application of mechanical force? Michael Sommer from Technische Universität Chemnitz, Michael Walter from Universität Freiburg, and their colleagues in Germany have synthesized and characterized a donor-acceptor (DA) torsional spring that undergoes planarization upon applying force, which results in shifts in absorption and emission spectra. In agreement with theoretical and experimental results, these features are reversible upon stress release. Currently, mechanochromic materials have limitations such as the need for two-state systems, lack of differentiation of forces, and nonreversibility. The researchers

describe their system as a DA mechanochromic torsional spring with a large dihedral angle in equilibrium geometry.

As reported in a recent issue of *Nature Communications* (<https://doi.org/10.1038/s41467-021-24501-1>), the organic molecules synthesized (DA) are substituted diphenyldiketopyrrolopyrroles (PhDPP), which are incorporated into an amorphous polyphenylene. One of the key characteristics of this system is the electronic communication; the molecules used have high electron densities that are distributed over the molecules. Also, there is a torsion angle present between the central diketopyrrolopyrrole moiety and the phenyl ring that attaches to the polymer. When planarization of the DA system occurs, the electronic communication is increased and angles change (torsion angle between moieties), which results in changes in the optical properties. The researchers attribute the planarization to the tendency of the DA system to increase π orbital overlap and reduced energy,

rather than the direct force acting on the spring (mechanical force).

The research team also carried out a substitution (*ortho* and *meta* in aromatic hydrocarbons) screening process to identify materials that rendered significant changes in optical properties. Steric hindrance from the substituents played a role by increasing torsion angle between rings. Results indicate that as force is applied and increased, the dihedral angle is reduced, and the maximum absorption wavelength is increased (redshift). Conversely, when force was released, the system returned to quasi-initial conditions, increasing the dihedral angle and decreasing the wavelength (hypsochromic shift). This was confirmed by a back-and-forth stress-strain experiment; the film was put in a mechanical system (Linkam TST-350) that elongated and shortened (negative elongation) the material resulting in a photoluminescence spectrum that showed wavelengths increasing and decreasing as positive and negative elongation occurred over time. In simple terms, the synthesized system can change color (and corresponding wavelength) depending on the amount of stress applied.

One of the major observations was the possibility of detecting geometric changes by optical changes, and detecting optical changes by geometric changes. The researchers predicted the quantitative change in wavelength per force applied to the system. In summary, the advantages of this DA system include fast response, reversibility, and continuous variation of wavelength with stress. This can lead to applications such as force sensor design, tamper-proof packing, and safety such as color change upon modifications in safety materials.

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(a) Stress versus time curve (black) of *ortho*-substituted diketopyrrolopyrrole during a stress-strain experiment with three relaxation breaks via negative elongation (5 mm min^{-1} for both directions). The corresponding shifts $\Delta\lambda_{\text{max,em}}$ (blue) from photoluminescence-spectroscopy were correlated to the stress values with time. (b) Images of the specimen under UV light (365 nm) at the four indicated positions in the stress-time curve. Credit: *Nature Communications*.

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