Computational Design, Synthesis, and Mechanochromic Properties of New Thiophene-Based π-Conjugated Chromophores

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The possibility of exploiting supramolecular architectures for the preparation of innovative mechanochromic devices has been extended by designing novel thienyl-substituted 1,4-bis(ethynyl)benzene dyes, which are characterized by a conjugated, rigid, rodlike core structure. This new family of chromophores was synthesized according to a simple two-step sequential cross-coupling reaction, and the optical properties were investigated in solution and in a polymeric matrix. To tune the mechanochromic performances in smart polymer materials, a virtual screening was set up that was able to select a derivative with optimal spectral features. The effective combination of experimental and computational investigations allowed us to spot those homologues with already potential anisotropic and aggregachromic features and characterized by the best spectral properties and luminescent response. The best candidate was synthesized and dispersed into a polyethylene matrix, indeed achieving an “in silico designed” mechanochromic material. Besides the specific applications of this novel material, the integration of computational and experimental techniques reported here defines an efficient protocol that can be applied to make a selection among similar dye candidates, which constitute the essential responsive part of such supramolecular devices.

Słowa kluczowe

chromophores, computational design, dyes/pigments, luminescence, mechanochromic materials

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