

TRIPHENYLAMINECONTAINING ASYMMETRIC THIAZOLOTHIAZOLE DERIVATIVES FOR PHOTONICS AND OLEDAPPLICATIONS

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Recent advances in optoelectronic materials have led to the identification of asymmetric thiazolothiazole (TT)-based fused heterocycles as a promising class of materials exhibiting attractive photophysical properties. Compared to symmetric analogues, improved tuning of electronic and optical properties is enabled in asymmetric TT derivatives through tailored donor–acceptor interactions, resulting in solvatochromism, enhanced luminescence efficiency, and balanced charge transport [1–3]. Structural asymmetry is further associated with the promotion of aggregation-induced emission enhancement and improved film morphology, thereby contributing to higher device efficiency and stability [4]. In this work, the design, synthesis, and characterization of asymmetric TT derivatives functionalized with triphenylamino, dimethylfluorenyl, and tetraphenylethenyl donor units at both terminals of the TT core are reported. High thermal and electrochemical stability, along with reversible oxidation behavior, is demonstrated by the synthesized compounds. Ionization energies of the films in the range of 5.48–5.58 eV are revealed by photoemission spectroscopy, indicating potentially favorable charge injection in OLED applications. Additionally, high charge carrier mobilities of up to $10^{-4} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ at an electric field of $1.6 \times 10^5 \text{ V cm}^{-1}$ are observed. The results of photophysical studies indicate strong potential for two-photon absorption [5] and OLED applications.

Keywords: Asymmetric Thiazolothiazole, Triphenylamine, OLEDs

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- [1] N. A. Sayresmith et al., "Photostable voltage-sensitive dyes based on simple, solvatochromic, asymmetric thiazolothiazoles," *J. Am. Chem. Soc.*, vol. 141, no. 47, pp. 18780–18790, 2019.
- [2] T. Ishi-i, K. Ikeda, M. Ogawa, and Y. Kusakaki, "Light-emitting properties of donor–acceptor and donor–acceptor–donor dyes in solution, solid, and aggregated states: structure–property relationship of emission behavior," *RSC Adv.*, vol. 5, no. 108, pp. 89171–89187, 2015.
- [3] A. N. Woodward et al., "Thiazolothiazole fluorophores exhibiting strong fluorescence and viologen-like reversible electrochromism," *J. Am. Chem. Soc.*, vol. 139, no. 25, pp. 8467–8473, 2017.
- [4] D. Zhang et al., "Triphenylamine/benzothiadiazole-based compounds for non-doped orange and red fluorescent OLEDs with high efficiencies and low efficiency roll-off," *J. Mater. Chem. C*, vol. 9, pp. 4921–4926, 2021.
- [5] R. R. Saputra et al., "A novel optical power-limiter-stabilizer candidate: Two-photon active chromophores derived from thiazolothiazole," *Asia-Pacific J. Sci. Technol.*, vol. 29, no. 2, p. 17, 2024.