

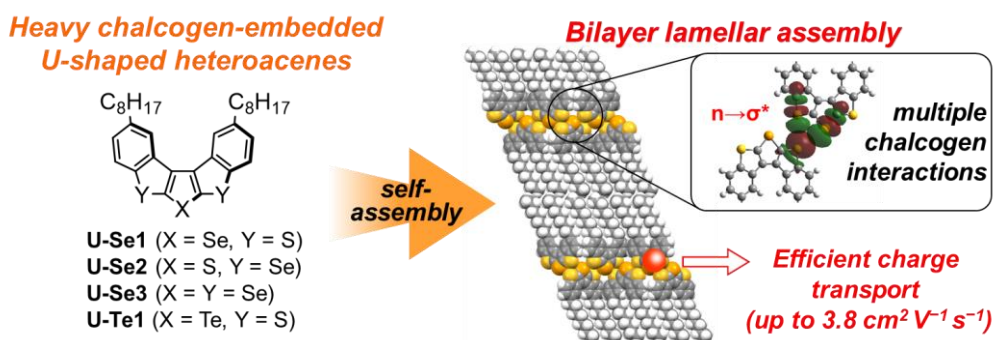
Development of Heavy Chalcogen-Embedded U-Shaped Heteroacenes Having Bilayer Self-Organization Capability

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Controlling the supramolecular assemblies of π -conjugated molecules is essential to achieve excellent functions such as charge carrier transport. One needs to carefully consider both π -cores and heteroatoms to fully exploit the material properties. Heteroatom-containing fused aromatic π -scaffold, referred to as heteroacenes, have been actively studied for high-performance organic semiconductors because their highly ordered molecular packing in the solid states maximizes the intermolecular electronic couplings to facilitate the charge transport. So far, most of the heteroacene-based materials showing excellent semiconducting properties adopted the linear-shaped π -cores with sulfur atoms. However, there are countless combinations of available π -cores and heteroatoms, offering opportunities to develop novel materials endowed with attractive properties.

In this work, we developed a new series of U-shaped heteroacenes featuring unconventional “U” geometric configuration embedded with chalcogen atoms (sulfur, selenium, and tellurium).^{1,2} The incorporation of heavier chalcogen atoms instead of sulfur effectively altered not only the basic optoelectronic properties but also the self-organization behaviors. Notably, U-shaped heteroacenes were found to form bilayer lamellar assemblies with a head-to-head arrangement, which is stabilized by the multiple intermolecular chalcogen interactions. High solvent solubility and crystallinity of U-shaped heteroacenes allowed us to apply them for a facile solution-based thin-film fabrication. Consequently, thin-film organic transistors based on selenium-embedded heteroacene exhibited high hole mobilities of up to $3.8 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. This work provided the advanced molecular design based on the U-shaped molecular configuration and strategic chalcogen substitution.^{1,2}



1) T. Mori, T. Yasuda, *Adv. Electron. Mater.* **2021**, in press.

2) T. Mori, T. Oyama, H. Komiyama, T. Yasuda, *J. Mater. Chem. C* **2017**, 5, 5872.