# Donor-acceptor-type organic semiconductors based on acenedichalcogenophenediones

([1]*Graduate School of Science, Tohoku University*, [2]*Center for Emergent Matter Science, RIKEN*) ○Kohsuke Kawabata,[1,2] Kazuo Takimiya,[1,2]

**Keywords**: donor-acceptor; organic semiconductor; quinoid; near-infrared absorption

Organic semiconductors having a small optical energy gap are of great interest for the application for near-infrared-active organic photovoltaics and photodetectors. For designing such materials, lowering LUMO energy levels is a key not only for reducing the energy gaps but also keeping low-lying frontier orbital energy levels for air stable carrier transport. We have recently developed a series of benzo- and naphtho-dithiophenediones as highly electron-deficient acceptor building units for D-A type conjugated oligomers[1] as well as polymers,[2] some of which exhibited very small optical energy gaps and low-lying frontier orbital energy levels. In this study, we have systematically synthesized thiophene-based D-A-D triads incorporating acenedithiophenedione acceptors and the corresponding oxygen- and selenium-containing analogues, namely, acenedifurandiones and acenediselenophenediones, respectively, to investigate the effect of the chalcogen atoms in the acceptors on the physicochemical properties (Fig. 1).

The D-A-D triads show intense absorption bands in visible to near-infrared region and low-lying frontier orbital energy levels, which enables ambient-stable hole and electron transport in the OFET devices. The electronic structures mostly depend on the size of acene cores and donors, but not on the chalcogen atoms, though some minor differences are observed between the oxygen-containing acceptors and the sulfur- and selenium-containing counterpart. In the presentation, we report the synthesis, structure, optical and electrochemical properties, and carrier transport properties of the series of D-A-D triad molecules, and discuss the structure-property relationships regarding the effect of the chalcogen atoms.

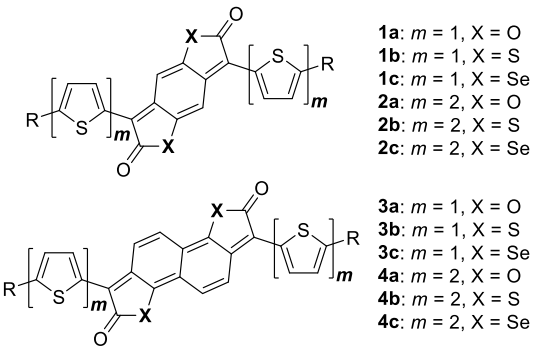


Fig. 1 Benzo- (top) and naphtho- (bottom) dichalcogenophenedione-based D-A-D triads.

1) K. Kawabata, I. Osaka, M. Sawamoto, J. Zafra, P. Burrezo, J. Casado, K. Takimiya, *Chem. Eur. J.* **2017**, *11*, 4579. 2) K. Kawabata, M. Saito, I. Osaka, K. Takimiya, *J. Am. Chem. Soc.* **2016**, *138*, 7725.