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## New p-azaquinodimethane core based narrow-gap non-ring fused organic acceptor†

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The design and synthesis of sAQM-1, a para-azaquinodimethane-based non-ring fused organic  $\pi$ -conjugated molecule with an undemanding, metal-free synthetic route, is reported. **sAQM-1** exhibits a narrow optical gap, stabilized frontier molecular orbitals, strong intramolecular charge transfer, and tunable self-assembly properties. Compared to the ring-fused Y6 acceptor, electronic energy levels are stabilized, and optical absorption red-shifted, demonstrating the potential of guinoidal scaffolds delivering atom economy and leading to narrow-gap organic electronic materials.

The rapid advancement in organic electronics has been fueled by solution processable  $\pi$ -conjugated organic molecules with highly tunable optoelectronic and structural features. These materials have found broad applications in electronics and photonics.<sup>2</sup> Among these, narrow-gap (<1.6 eV) organic semiconductors are of interest for organic photovoltaics (OPVs),<sup>3</sup> photodetectors (OPDs),4 and field-effect transistors (OFETs),5 as they exhibit extended light absorption into the near-infrared (NIR) region in which the NIR photons can be harvested or detected.3,6

A common design strategy for narrow-gap materials employs a donor-acceptor (D-A) approach. In this method, donor and acceptor moieties alternate within a  $\pi$ -conjugated backbone, inducing intramolecular charge transfer (ICT), contributing to a quinoidal character and formation of newly hybridized frontier molecular orbitals (Fig. 1(a)).5 This strategy is further enhanced by increasing molecular coplanarity through ring fusion and non-covalent interactions, improving molar absorptivity and charge-carrier mobility.<sup>6–8</sup>

Fig. 1 (a) Donor-acceptor system demonstrating intramolecular charge transfer (ICT). (b) Quinoid (left) and benzenoid (right) resonance forms of para-quinodimethane (p-QM). (c) Resonance configuration of mixed aromatic/quinoid structures, where Q and Ar indicates quinoidal and aromatic moieties, respectively, and examples structures.

Another alternative strategy is to utilize quinoid molecules, which feature double bonds between the two adjacent molecules, forcing coplanarity within the molecular backbone.<sup>9,10</sup> However, classical quinoidal units such as para-quinodimethane (p-QM, Fig. 1(b)) suffer from poor ambient stability due to a tendency to adopt reactive open-shell aromatic diradical (benzenoid) forms, which are more energetically favorable than the quinoidal form. 11 This challenge of reactivity can be overcome by stabilizing the quinoidal form by incorporating electron-withdrawing groups or embedding the quinoidal moiety within the  $\pi$ -conjugated backbone. <sup>12</sup> For the latter, there

a) Donor-Acceptor D b) Quinoidal c) Quinoidal Resonance Stabilization (Ar Tricyclic

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is a balance between the quinoidal and aromatic forms within the conjugated structure (Fig. 1(c)). 13-15 Quinoidal molecules and polymers based on this strategy have been reported and demonstrated exceptional NIR absorption and structural stability. Examples include polycyclic heteroquinoid groups such as benzodifurandione (O), 16-18 benzodipyrrolidone (N-R), 19-22 benzodithiophenedione (S), 23-25 or oxindole-capping, 26-28 and others (Fig. 1(c)). 15,29

Research Article

In 2017, Liu et al. introduced p-azaquinodimethane (p-AQM), an ambient-stable quinoidal unit.30 The stability was established by incorporating heteroatom (nitrogen) and alkoxy group into a p-QM scaffold, along with flanking aromatic units (Fig. 2(a)). Additionally, p-AQM offers a simple and scalable synthetic route via Knoevenagel condensation, avoiding a metal-catalyzed crosscoupling reaction. 31,32 While p-AQM has shown promise in creating narrow-gap polymers for applications such as OFETs, 30,33-36 and photothermoelectric devices, 32,37 its potential to afford narrow-gap molecules remains largely unexplored. The broader chemistry of p-AQM and its versatility in tuning electronic properties has recently been comprehensively reviewed, further providing its relevance in organic electronics.38

One of the state-of-the-art narrow-gap molecules is Y6 (Fig. 2(b)). This A-D-A'-D-A type fused-ring acceptor has demonstrated exceptional performance in OPVs and OPDs. 39,40 However, synthetic complexity has become a significant hindrance. Multiple organometallic coupling reactions and demanding ring-fusing steps increase production costs and limit scalability. 41 Therefore, the development of non-ring fused molecular acceptors has emerged as an important strategy. 42-47

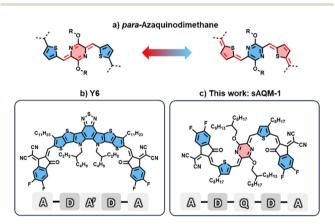


Fig. 2 (a) Quinoid-aromatic resonance forms of para-azaquinodimethane (p-AQM), chemical structures of (b) Y6 and (c) this work: sAQM-1

This work presents a non-ring fused p-AQM-based acceptor, sAQM-1, with an A-D-Q-D-A type structure (Fig. 2(c)). The stabilized quinoidal resonance form of p-AQM enables ambient stability, endowing a narrow optical and electrochemical gap while affording a simple atom-economical synthesis.

sAQM-1 was obtained in a metal-free, four-step synthetic route, as shown in Scheme 1. Commercially available 1,4diacetylpiperazine-2,5-dione was subjected to Knoevenagel condensation reaction with 4-octylthiophene-2-carboxaldehyde, yielding compound (1) with a 39% yield. The low yield is attributed to the impure starting material containing 10% isomer (3-octylthiophene-2-carboxaldehyde). Compound (1) was then subjected to an O-alkylation reaction using 2-hexadecyl bromide under mild basic conditions, affording compound (2) with an 84% yield. This was followed by a Vilsmeier-Haack formylation reaction to obtain compound (3) with a 75% yield. It should be noted that without the side chain on the thiophene moiety, the O-alkylated product exhibits topochemical activity, undergoing heat- or light-induced solid-state polymerization. This behavior aligns with reports of p-AQM molecules that undergo topochemical polymerization depending on the extent of end-group aromaticity,<sup>48</sup> end-group substituents,<sup>49</sup> and the proximity of reactive methylene groups.<sup>50</sup> In this case, installing a side chain on the thiophene suppresses such reactivity. Finally, sAQM-1 was obtained through a Knoevenagel condensation reaction between compound (3) and the endcap, 2-(5,6difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene) malononitrile, yielding the final product with a 93% yield. The chemical structure of sAQM-1 was fully characterized using 1H and <sup>13</sup>C NMR spectroscopy, high-resolution mass spectrometry, and CHN elemental analysis (Fig. S7, S8, S12 and S13, ESI†). Details about the synthesis and characterizations for each compound are available in ESI.†

Thiophene-flanked p-AQM has been reported to favor intramolecular S...N interactions, enhancing coplanarity by reducing rotational freedom.30 Additionally, the introduction of additional vinylic bridges, such as those from the endcap, can further enhance backbone planarity.<sup>33</sup> To probe the molecular conformation of sAQM-1, a variable-temperature (VT) <sup>1</sup>H-NMR spectroscopic experiment was performed in 1,1,2,2tetrachloroethane-d<sub>2</sub> (Fig. S14 and S15, ESI†). As the temperature increased from 21 °C to 120 °C, all resonances shifted upfield. Additionally, no broadening or coalescence was observed. The observed upfield shift is attributed to the disruption of intermolecular interactions rather than intramolecular rotation. Although the VT-1H NMR spectroscopic experiment does not provide direct insight into the molecular



Scheme 1 Synthesis schematics for sAQM-1. (i) NEt<sub>3</sub>, DMF, 120 °C, overnight (39%), (ii) K<sub>2</sub>CO<sub>3</sub>, DMF, 120 °C, 2.5 hours (84%), (iii) POCl<sub>3</sub>, DMF, CH<sub>2</sub>Cl<sub>2</sub>, 65 °C, 16 hours (75%), (iv) pyridine, CHCl<sub>3</sub>, 65 °C, overnight (93%)

conformation of **sAQM-1**, the absence of spectral changes suggests that it adopts a fixed and rigid conformation across all temperatures, unlike non-ring fused molecules with rotatable single C–C bonds. The density functional theory (DFT) calculations also show that the S···N non-covalent interaction in the Z,Z isomer leads to a more favorable conformation, which is more stable than the E,E isomer, in line with the literature (Fig. S16, ESI $\dagger$ ).  $^{30,31}$ 

Owing to the structural rigidity, sAQM-1 has lower solubility than expected. Nevertheless, it can be solubilized in solvents such as chlorobenzene, chloroform, o-dichlorobenzene, and o-xylene upon heating at 65 °C at 5 mg mL<sup>-1</sup>. However, the compound forms needle-like crystallites over time when returned to room temperature, demonstrating a tendency to aggregate (Fig. S17, ESI†). To further study intermolecular interactions of sAQM-1, concentration-dependent <sup>1</sup>H-NMR was performed in CDCl<sub>3</sub> (Fig. S18 and S19, ESI†). As the concentration increases from 0.5 to 5 mg mL<sup>-1</sup>, the aromatic protons are shifted downfield, while aliphatic protons show no obvious change. The downfield shift of aromatic protons is attributed to the ring current effects resulting from the increased  $\pi$ - $\pi$  stacking interactions, <sup>52</sup> with methylene proton adjacent to the p-AQM core showing the most prominent shift at about 0.07 ppm, indicating extensive intermolecular interactions (Fig. S18, ESI†).

The thermal behavior of **sAQM-1** was determined using differential scanning calorimetry (DSC, Fig. S20 and S21, ESI†) and compared to **Y6**. The first heating of **Y6** exhibits a sharp endothermic melting point ( $T_{\rm m}$ ) at 294.5 °C, consistent with previous reports (Fig. S20a, ESI†). <sup>53,54</sup> In contrast, the cooling scan of **Y6** shows no distinct exothermic crystallization peak ( $T_{\rm c}$ ), likely due to its slow crystallization kinetics arising from the large fused backbone and complex molecular structure. <sup>55,56</sup> As a result, the second DSC cycle of **Y6** shows no thermal transition (Fig. S21a, ESI†). For **sAQM-1**, the second DSC cycle displays sharp endothermic and exothermic transitions at 222.6 °C and 205.0 °C, respectively (Fig. S21b, ESI†). These distinct transitions indicate that **sAQM-1** possesses high structural rigidity. Such behavior is similar to related molecules with D-A structures incorporating conformational locks. <sup>57-59</sup>

The electronic properties of **sAQM-1** were examined using solution cyclic voltammetry (CV) in  $\mathrm{CH_2Cl_2}$  and compared to **Y6** (Fig. 3(a), Fig. S22 and Table S1, ESI†). Note that solution CV has resulted in discrepancies with **Y6** energy levels from the literature, as they are reported using CV in film.<sup>39</sup> **Y6** exhibits an irreversible first reduction process, whereas **sAQM-1** shows reversible reduction. Conversely, the first oxidation process is reversible for **Y6** and quasi-reversible for **sAQM-1**. The first reduction occurs at -0.93 V ( $E_{\mathrm{onset}}^{\mathrm{red}}$ ) for **Y6** and -0.77 V ( $E_{\mathrm{1/2}}^{\mathrm{red}}$ ) for **sAQM-1** ( $\nu$ s. Fc/Fc<sup>+</sup>), while the oxidation occurs at 0.61 V ( $E_{\mathrm{1/2}}^{\mathrm{ox}}$ ) for **Y6** and 0.59 V ( $E_{\mathrm{onset}}^{\mathrm{ox}}$ ) for **sAQM-1** ( $\nu$ s. Fc/Fc<sup>+</sup>).

The optical properties of **sAQM-1** were studied by optical absorption spectroscopy and directly compared with **Y6** (Fig. 3(b)). In CHCl<sub>3</sub> solution, both **Y6** and **sAQM-1** exhibit sharp vibronic peaks (0-0 and 0-1) in the low-energy absorption band.<sup>60</sup> The absorption peaks for **Y6** are located at 734 and

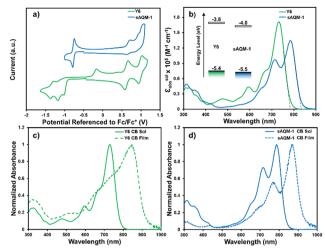


Fig. 3 (a) Cyclic voltammogram of Y6 (green) and sAQM-1 (blue). CVs were measured in  $CH_2Cl_2$  solution under  $N_2$  referenced to the Fc/Fc<sup>+</sup> couple (Fc: ferrocene), recorded at 100 mV s<sup>-1</sup>. (b) Absorption spectra of Y6 and sAQM-1 solution in CHCl<sub>3</sub> (CF). (Inset) Energy level diagram of Y6 and sAQM-1. Normalized optical absorption spectrum of (c) Y6 and (d) sAQM-1 chlorobenzene (CB) solution (solid line) and annealed chlorobenzene (CB) spin-cast film at 150 °C for 10 minutes (dotted line).

672 nm, respectively, with a molar extinction coefficient ( $\epsilon_{\rm abs}^{\rm sol}$ ) of 1.7  $\times$  10<sup>5</sup> M<sup>-1</sup> cm<sup>-1</sup>, while **sAQM-1** exhibits peaks at 782 and 714 nm, respectively, with  $\epsilon_{\rm abs}^{\rm sol}$  of 1.3  $\times$  105 M<sup>-1</sup> cm<sup>-1</sup> (Fig. S23 and S24, ESI†). The presence of sharp vibronic peaks and relatively high  $\epsilon_{\rm abs}^{\rm sol}$  suggest that both molecules maintain a rigid and planar conformation in solution, resulting in enhanced intermolecular interactions and ICT effect. <sup>61</sup> **sAQM-1** has a narrower optical gap ( $E_{\rm g}^{\rm opt}$ ) than **Y6**, with the 0-0 peak and absorption onset red-shifted relative to **Y6** by 51 nm and 48 nm, respectively.

The calculated energy gap  $(E_{\rm g}^{\rm CV})$  follows the same trend as  $E_{\rm g}^{\rm opt}$ , supporting that **sAQM-1** has a narrower gap than **Y6**. Using  $E_{\rm 1/2}^{\rm ox}$  value (or  $E_{\rm LUMO}-E_{\rm g}^{\rm opt}$ , if oxidation is not reversible), the highest occupied molecular orbital energy level  $(E_{\rm HOMO})$  was estimated to be -5.4 eV for **Y6** and -5.5 eV for **sAQM-1** (Fig. 3(b)). The lowest unoccupied molecular orbital energy level  $(E_{\rm LUMO})$  was estimated using  $E_{\rm 1/2}^{\rm red}$  value (or  $E_{\rm HOMO}+E_{\rm g}^{\rm opt}$ , if reduction is not reversible), yielding -3.8 eV for **Y6** and -4.0 eV for **sAQM-1** (Fig. 3(b)). Overall, **sAQM-1** exhibits more stabilized frontier molecular orbital energy levels and a smaller energy gap than **Y6**, thus indicating that the quinoidal conjugation strategy is effective at mimicking the properties of ring-fused systems. The optoelectronic data are summarized in Table 1.

The photoluminescence (PL) spectra of **Y6** and **sAQM-1** were measured in chlorobenzene (CB), chloroform (CF), dichlorobenzene (o-DCB), and o-xylene (Fig. S25, ESI†). Both molecules exhibit polarity-dependent absorption and emission, indicative of a strong ICT effect.<sup>62</sup> The Stokes shift, which represents the energy loss during the transition between the ground and excited states, was calculated from the difference between maximum absorption ( $\lambda_{\text{max}}^{\text{sol}}$ ) and emission energies (Table S2, ESI†).

Table 1 Experimental optoelectronic properties of Y6 and sAQM-1

	Absorption spectra			Cyclic voltammetry			Energy level	
Compound	$\lambda_{\max}^{\text{sol}}{}^a$ [nm]	$\lambda_{\mathrm{onset}}^{\mathrm{sol}}{}^{b}$ [nm]	$E_{\rm g}^{{ m opt}c}$ [eV]	Ered [V]	$\begin{array}{c} E_{1/2}^{\rm ox} \\ {\rm [V]} \end{array}$	$E_{\mathrm{g}}^{\mathrm{CV}d}$ [eV]	E <sub>LUMO</sub> <sup>e</sup> [eV]	E <sub>HOMO</sub> <sup>f</sup> [eV]
Y6	734	784					-3.83	
sAQM-1	782	832	1.49	-0.77	$0.59^{g}$	1.36	-4.03	-5.52

<sup>a</sup> Absorption maximum in chloroform solution ( $\sim 10^{-5}$  M). <sup>b</sup> Onset absorption edge of solutions. <sup>c</sup> Optical bandgap calculated from the onset absorption edge of solutions, calculated by  $E_{\rm g}^{\rm opt} = 1240/\lambda_{\rm onset}^{\rm sol}$ . Energy bandgap calculated from solution cyclic voltammetry using the first  $E_{1/2}$  or  $E_{\rm onset}$  values for reduction and oxidation.  $^e$  Calculated by  $E_{\rm LUMO} = -4.8$  eV  $-E_{1/2}^{\rm red}$ , if not reversible,  $E_{\rm LUMO} = E_{\rm HOMO} + E_{\rm opt}^{\rm opt}$ . f Calculated by  $E_{\text{HOMO}} = -4.8 \text{ eV} - E_{1/2}^{\text{ox}}$ , if not reversible,  $E_{\text{HOMO}} = -4.8 \text{ eV}$  $E_{
m LUMO}$  –  $E_{
m g}^{
m opt}$ .  $^g$  Indicates for the  $E_{
m onset}$  value for the reduction or oxidation due to their quasi-reversibility or irreversibility.

sAQM-1 had smaller Stokes shift compared to Y6 by 0.04, 0.01, 0.06, and 0.04 eV in CB, CF, o-DCB, and o-xylene, respectively, suggesting a lower energy loss through nonradiative decay, again, likely due to a more rigid molecular conformation. Smaller excited-state relaxation correlates with reduced reorganization energy, which can enhance exciton lifetime and diffusion length.63

Y6 films spin-casted from CB solutions show significantly broadened absorption and a ~100 nm redshift in the 0-0 peak after annealing (Fig. 3(c)). This broadening is attributed to multiple packing modes between the end groups and units.64 These packing interactions facilitate the formation of a 3D network, resulting in enhanced charge transport in multiple directions. 65,66 In contrast, annealed sAQM-1 spin-casted films from CB show sharp, red-shifted vibronic peaks at 0-0 and 0-1 by  $\sim$  83 and 52 nm, respectively, without significant broadening (Fig. 3(d) and Fig. S26, ESI†). The high 0-0/0-1 ratio combined with red-shifted absorption suggests enhanced  $\pi$ - $\pi$ intermolecular interactions and dominant J-type aggregation in the solid state, while minimal broadening indicates the lack of variation in packing modes.67

Notably, sAQM-1 exhibits drastically different self-assembly behavior when processed from CF. The as-cast film shows a low 0-0/0-1 transition ratio, with the 0-0 and 0-1 peaks at  $\sim$  857 nm and ~743 nm, respectively. Upon annealing up to 120 °C, the 0-0/0-1 ratio increases (Fig. S27, ESI†). However, at a higher temperature, the 0-0 peak and absorption onset are slightly blue shifted by  $\sim 15$  nm, and a new peak appears at 630 nm (Fig. S27, ESI†). These observations suggest that sAQM-1 may adopt an H-aggregated structure. The aggregation type can be tuned using solvent additives during the film forming and annealing process. For example, adding 1% CB or 1-chloronaphthalene (CN) additives in CF solution during film formation promotes J-aggregation, giving a red-shifted optical profile, 1% 1,8-diiodooctane (DIO) and diphenyl ether (DPE) has no noticeable effects (Fig. S28, ESI†). Therefore, this smart solvent addition presents a unique opportunity to control molecular self-assembly.

Synchrotron-based grazing-incidence wide-angle X-ray scattering (GIWAXS) analysis further supports this observation, as

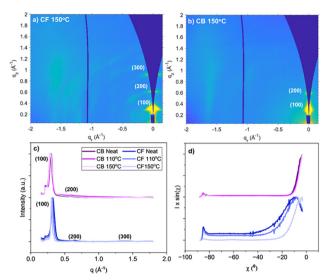


Fig. 4 (a) and (b) 2D GIWAXS patterns ( $\theta = 0.15^{\circ}$ ) for **sAQM-1** films cast from (a) CF and (b) CB, after annealing at 150 °C. (c) Corresponding azimuthally integrated diffraction patterns. (d) Azimuthal ( $\chi$ ) linecut profiles for CF- and CB-cast films, integrated over a q range of 0.2–0.4  ${ t Å}^{-1}$ 

demonstrated by the 2D scattering pattern (Fig. 4(a) and (b)), azimuthally integrated diffraction profiles (Fig. 4(c)), and  $\chi$ dependent linecut profiles (Fig. 4(d)). In these experiments, sAQM-1 was spin-coated onto silicon substrates at 3000 rpm from either CB or CF solutions. The resulting films were analyzed in their as-cast (neat) state or after thermal annealing at 110 °C or 150 °C for 10 minutes.

The scattering spectra reveals that films are moderately semicrystalline, with both exhibiting a dominant, highintensity (100) reflection at approximately  $q = 0.2 \text{ Å}^{-1}$ . Films cast using CB show tendency for increased interplanar spacing  $(d_{100} \approx 21.36 \text{ Å})$  compared to those cast with CF  $(d_{100} \approx 20.05 \text{ Å})$ (Table S3, ESI†). Additionally, CF-cast films exhibit multiple packing modes ( $q_{200}$  and  $q_{300}$ , Fig. 4(a) and (b)) that are more disordered than those observed in CB-cast films. This is better illustrated in Fig. 4(d), where the broadening of the high-intensity peak at  $\chi = -8^{\circ}$  for CF films indicates mixed orientations within the (100) packing structure. Upon annealing, this distribution narrows, suggesting that increased thermal treatment promotes more ordered molecular packing (Fig. S29, ESI†). In contrast, CBcast films display a narrower distribution consistent with a single preferred orientation, aligning with the absorption spectra that shows minimal variation in the packing modes and orientations of sAQM-1 when processed with CB.

Electron mobility was measured using electron-only devices to evaluate the electron transport properties of sAQM-1. Although sAQM-1 may indicate superior performance when processed in solvents such as CB and o-xylene, CF and CF + 1 vol% CB were selected to ensure consistency in film thickness and compatibility with the processing conditions used for the benchmark material, Y6, cast from CF. 39,68 Electron mobility was extracted by analyzing the dark J-V characteristics using the Murgatroyd relation for the single-carrier space charge limited current (SCLC) method:

$$J_{\rm SCL} = \frac{9}{8} \, \varepsilon_{\rm r} \varepsilon_0 \mu \, \frac{V^2}{L^3} {\rm exp} \bigg( \frac{0.89 \beta}{\sqrt{L}} \sqrt{V_{\rm in}} \bigg)$$

where  $J_{\text{SCL}}$  is the current density,  $\mu$  is the carrier mobility,  $\varepsilon_{\text{r}}$  is the relative permittivity,  $\varepsilon_0$  is vacuum permittivity, L is the thickness of the device, and  $\beta$  is the field activation factor. 69-71 Since film thickness influences mobility, electrononly devices were fabricated using two spin speeds, 1000 rpm (1k) and 2000 rpm (2k), for both Y6 and sAQM-1 to enable a consistent comparison. The corresponding film thicknesses for each condition are provided in Table S4 in the ESI.† As shown in Fig. 5(a), the benchmark material Y6 exhibits an average electron mobility of around 1  $\times$  10<sup>-4</sup> cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> to 1  $\times$  $10^{-5}~\text{cm}^2~\text{V}^{-1}~\text{s}^{-1}$ , consistent with the values reported in the literature. 39,68 In comparison, sAQM-1 devices show relatively lower initial electron mobility of around  $5 \times 10^{-7}$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> for devices processed in CF and between  $10^{-7}$  and  $10^{-8}$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> for devices processed in CF + 1 vol% CB. Interestingly, after illumination, the electron mobilities of sAQM-1 increased significantly to about 2 imes  $10^{-5}$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> for devices processed in CF and between 10<sup>-6</sup> and 10<sup>-7</sup> cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> for devices processed in CF + 1 vol% CB, representing an improvement of about two orders and one order of magnitude, respectively (Fig. 5(b)). In contrast, the increase in mobility for Y6 was less than one order of magnitude. This is confirmed with at least 5 different devices, as shown in Fig. S30 (ESI†), with the best and average values shown in Table S4 (ESI†). This enhancement in mobility for sAQM-1 can be attributed to light soaking effect, commonly observed in metal oxides like SnO<sub>2</sub>, <sup>72,73</sup> and interaction between SnO<sub>2</sub> and sAQM-1 layer, which may be unfavorable in the fresh device state. This pronounced improvement in sAQM-1 electron mobility suggests that with further optimization in structural modifications, processing, and solid-state properties, this molecular scaffold has the potential to achieve high mobilities comparable to Y6 in the fresh state. Furthermore, the higher mobility of sAQM-1 processed in CF suggests the H-aggregated structure, in this case, may lead to better electronic performance.

In conclusion, this work presents the design and synthesis of **sAQM-1**, a quinoidal non-ring fused small-molecule based on

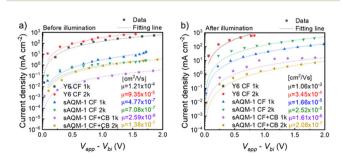


Fig. 5 Dark J-V characteristics of electron-only devices based on **Y6** and **sAQM-1** for electron mobility extraction using the modified Mott–Gurney law (SCLC method): (a) before and (b) after continuous illumination at 100 mW cm $^{-2}$  for 18 hours in a nitrogen environment. **Y6** and **sAQM-1** layers for devices were processed in CF and CF + 1 vol% CB using two different spin speeds: 1000 rpm (1k) and 2000 rpm (2k).

p-AQM core, using a simple and metal-free four-step synthesis route. sAQM-1 exhibits optoelectronic properties similar to the state-of-the-art fused-ring acceptor Y6, including a narrow optical and electrochemical gap. Structural characterization suggests that sAQM-1 adopts a rigid and planar conformation with strong intermolecular interactions and structural rigidity, attributed to a stabilized quinoidal resonance form and conformational locks. The aggregation mode can be tunable through a careful selection of solvents and additives. Overall, this study demonstrates the potential of stabilized quinoidal cores like p-AQM as versatile scaffolds to create near-IR absorbing molecules. Future work will focus on structural tuning to further modulate energy levels, solubility, and self-assembly properties, with the goal of achieving anisotropic charge transport, like Y6, with potential applications in organic photodetectors, photovoltaics, and related optoelectronic devices.

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#### Conflicts of interest

There are no conflicts to declare.

#### Data availability

The data supporting this article have been included as part of the ESI.† This data includes NMR spectra, mass spectra, elemental analysis data sheets, DSC plots, and mobility data.

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