ALDRICH Materials Science

Highly Absorbing Squaraines and Their Application to Organic Photovoltaics

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Organic Photovoltaics (OPVs) have attracted a great deal of research interest as they are potentially low cost, lightweight, and flexible sources for renewable energy. Exploring new materials is one of the critical approaches to achieve high-performance OPVs in solar cell research. This article describes squaraine dyes as highly efficient absorbers for OPV applications.

Squaraines are 1,3 derivatives of squaric acid, a condensation product of squaric acid and electron-rich aromatics or heterocycles. Squaraine dyes feature sharp and intense solution absorption in the red to near infrared (NIR) region of the solar spectrum. More importantly, squaraine film absorption is quite broad, which is highly beneficial for sunlight absorption. A series of novel, high purity squaraines have recently been prepared, including the products in the table below.[1] 2,4-bis[4-(*N*,*N*-diisobutylamino)-2,6-dihydroxyphenyl] squaraine (SQ, **Aldrich Prod. No. 758337**) has been successfully utilized as a donor material for high-performance cells in both vacuum-deposited and solution-processed OPVs.[2] Pairing SQ with PC_{70}, C_{70}-fullerene acceptor, has achieved high power conversion efficiency of 5.5% mainly due to its high open circuit voltage, high short circuit current, and high fill factor.[3] Replacing diisobutylamino substituents with diphenyl amino moieties, 2,4-bis[4-(*N*,*N*-diphenylamino)-2,6-dihydroxyphenyl] squaraine (DPSQ, **Aldrich Prod. No. 757233**), improved solubility for solution-processing of OPVs with enhanced charge carrier mobility. DPSQ, with its 0.2 eV deeper HOMO energy than SQ, is anticipated to lead to OPV devices with higher open circuit voltage and hence better device performance (Figure 1).[4]

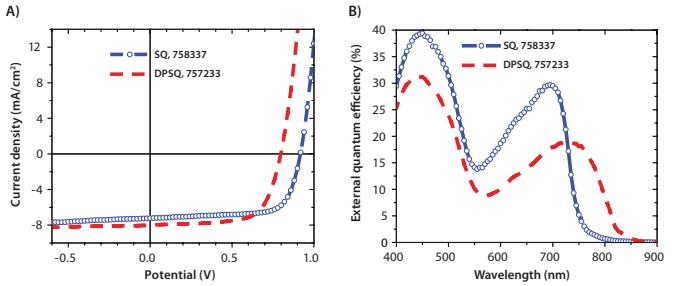

Figure 1. A) current density (*J*) versus voltage (*V*) characteristics at 1 sun illumination of the as-cast SQ/C_{60} and DPSQ/C_{60} cells with structure of ITO/MoO3(80 Å)/SQs(85 ± 5 Å)/C_{60}(400 Å)/3,4,9,10 perylenetetracarboxylic bisbenzimidazole (PTCBI) (80 Å)/Ag (1,000 Å) and **B)** External quantum efficiencies (*EQE*) plot.

In summary, initial studies of these squaraine derivatives utilized as absorbers in OPV devices showed enhanced charge carrier mobility and higher open circuit voltage, compared to previously studied squaraines. Further optimization of device performance using this class of small molecules is in progress.

References

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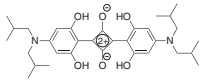
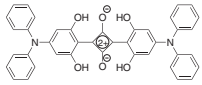
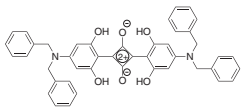
(2) Wang, S. Y.; Mayo, E. I.; Perez, M. D.; Griffe, L.; Wei, G. D.; Djurovich, P. I.; Forrest, S. R.; Thompson, M. E., *Appl. Phys. Lett.*, **2009**, *94*, 233304.
(3) Wei, G. D.; Wang, S. Y.; Sun, K.; Thompson, M. E.; Forrest, S. R., *Adv. Energy Mater.*, **2011**, *1*, 184.
(4) Wei, G. D.; Xiao, X.; Wang, S. Y.; Sun, K.; Bergemann, K. J.; Thompson, M. E.; Forrest, S. R., Manuscript in preparation., **2011**.

Description	Structure	Prod. No.
2,4-bis[4-(*N*,*N*-diisobutylamino)-2,6-dihydroxyphenyl] squaraine (SQ)		**758337-1G**
2,4-bis[4-(*N*,*N*-diphenylamino)-2,6-dihydroxyphenyl] squaraine (DPSQ)		**757233-1G**
2,4-bis[4-(*N*,*N*-dibenzylamino)-2,6-dihydroxyphenyl] squaraine (DBSQ)		**757268-1G**

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