Electronic Supplementary Information (ESI)

Synthesis of visible-light-absorptive and hole-transporting periodic mesoporous organosilica thin films for organic solar cells

Masamichi Ikai,‡,a,b,c Yoshifumi Maegawa,‡,a,b,c Yasutomo Goto,a,b,c Takao Tani a,b and Shinji Inagaki*,a,b,c

a Toyota Central R&D Labs., Inc., Nagakute, Aichi 480-1192, Japan
b Core Research and Evolution Science and Technology (CREST), Japan Science and Technology Agency (JST), Japan
c Advanced Catalytic Transformation program for Carbon utilization (ACT-C), Japan Science and Technology Agency (JST), Japan

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‡ M. I. and Y. M. equally contributed to this article.
* Corresponding author, E-mail: inagaki@mosk.tytlabs.co.jp
Figure S1. (a) $^1$H NMR and (b) $^{13}$C NMR spectra of organosilane precursor 1 in CDCl$_3$. 
Figure S2. (a) $^1$H NMR and (b) $^{13}$C NMR spectra of organosilane precursor 2 in CDCl$_3$. 
**Krypton adsorption–desorption isotherms**

Krypton adsorption–desorption isotherms were measured using a Quantachrome Autosorb-1 at 87 K. The films (1-PMO-F) were formed on 16 cleaned glass substrates (24 mm×32 mm×0.15 mm) by spin-coating sol C and extracting templates. The total weight of 1-PMO-F (16 pieces) was 0.31 mg. The samples were sliced into pieces and placed in a special cell for the measurements of isotherms.

Figure S3 shows a krypton adsorption–desorption isotherm of 1-PMO-F on glass substrates. The Brunauer–Emmett–Teller (BET) surface area was calculated to be 285 m$^2$ g$^{-1}$.

From SEM images of 1-PMO-F, we estimated the number of mesopores with a diameter of 15 nm to be 18 in a unit cell of (50×50×50) nm$^3$. Using this information and the weight of 1-PMO-F measured (0.31 mg), we estimated that the surface area is 225 m$^2$ g$^{-1}$. There is no large difference between the value obtained from the experiment and the estimated value.

![Figure S3](image-url). Krypton adsorption–desorption isotherm of 1-PMO-F.
**Pore size distribution of mesopores**

We analyzed the pore size distribution for mesopores in top-view SEM images of 1-PMO-F using an image analysis software. Figure S4 shows pore size distribution of mesopores. Three different SEM images were used (analyzed area: 1.1 \( \mu m^2 \)).

From this analysis, we obtained the average pore size for mesopores and its standard deviation. Those values are 15 and 4 nm, respectively. The coefficient of variation (standard deviation / average pore diameter) is about 0.28. The value is similar to that (0.22*) of a conventional PMO film which was estimated by the pore size distribution curve derived from nitrogen adsorption.16

(* The value of 0.22 was estimated from inset data of Fig. S7 in ESI (reference 16).)

![Figure S4](image)

*Figure S4.* Pore size distribution of mesopores for 1-PMO-F. Three different Top-view SEM images were analyzed.
**Figure S5.** Normalized absorbance of both 1-NP-F (blue) and 2-NP-F (red) films.

**Figure S6.** EQE of the 1-PMO-F based solar cell (black, solid), and normalized absorbance of both 1-PMO-F (blue, solid) and PCBM (blue, dashed) films.
Figure S7. Ionization potentials of 1-NP-F and 2-NP-F measured by using AC-2.
Figure S8. $J-V$ characteristics of (a) device A or (b) device B without a buffer layer (black lines) and with 1'-NP-F buffer layer (red lines) in the dark (broken lines) and under 1 sun, AM1.5 illumination (solid lines).