Supplementary Information

Solution-Processed Blue Phosphorescent Organic Light-Emitting Diodes Using a Ge-Based Small Molecular Host

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Theoretic Calculations

In order to test the accuracy of the calculation results, we first compared the results of FIrpic against known experimental values. As shown in Table S1, the calculated HOMO energy (−5.86) for FIrpic based on B3LYP/6-311++G(d,p) level is identical to the experimental value of −5.8 eV. The calculated triplet energy (E_T) is also in reasonable agreement with the experimental result of 2.7 eV. And the calculated dipole moment (μ) shows a high view of 6.53 Debye, which indicated that FIrpic should be soluble in an alcohol, and this is identical to the experimental phenomenon. From these results,[S1] the B3LYP/6-311++G(d,p) method can be regarded as a reasonable method for these calculations.

Relative Quantum Yield Measurement

The UV-vis absorption and PL spectra of DCzGe and POPOP in cyclohexane were shown in Fig. S2. In order to improve the precision of quantum yield measurement, the solution of DCzGe and POPOP were prepared by controlling the absorption optical density around 0.05 at 300 nm in cyclohexane. The final absorption optical density of DCzGe and POPOP were 0.046 and 0.045 respectively, and the relative PL integrated intensity were 79 500 and 129 691 excited by 300 nm. The absolute quantum yield of POPOP is 97% excited by 300 nm in cyclohexane.[S2,S3] The relative quantum yield is calculated using :

$$Q = Q_R \frac{I \; OD_R n^2}{I_R \; OD \; n_R^2}$$

In this equation Q is the quantum yield, I is the integrated intensity, n is the refractive index, OD is the optical density. The subscript R refers to the reference fluorophore of known quantum yield.

Cross-section Image

The SEM cross-section image of PVK/EML was depicted in Figure S3. The PVK/EML film, fabricated

with the same method as used for device 5, was spin-coated on the top of PEDOT:PSS-coated Si/SiO$_2$ slide. A silver layer was evaporated on this film to confirm the cross-section structure of the organic film when fabricating the sample.

Characterization of device without OXD-7

The device without electron transport material (OXD-7) (ITO/PEDOT:PSS/PVK/DCzGe:FIrpic/Ca/Al) was also fabricated, using the same processing method with device 5, but this device showed a poor performance. The maximum luminance was only about 90 cd/m^2. When the voltage increased to 27.5 V, the device was broken down. This is mainly due to the lack of sufficient pathways for electrons in the device, so lots of electrons were blocked at the interface between the emitting layer and the cathode, leading to the weak luminance. As a result, in our devices (1−6) OXD-7 was introduced for obtaining better luminous performance, which is a commonly-used strategy for Si-based host materials[S4] and other *p*-type host materials.[S5]

Table S1 Calculated energies and dipole moment for FIrpic and designed molecules.

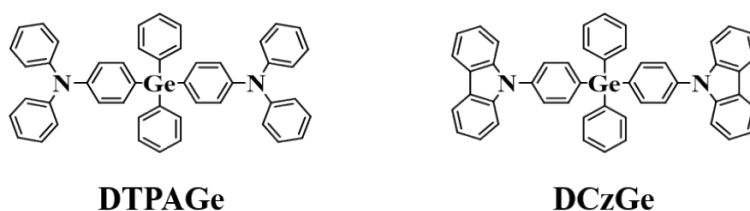|	HOMO [eV]	LUMO [eV]	E_T [eV]	V_{IP} [eV]	V_{EA} [eV]	μ [Debye]
FIrpic	-5.86	-2.22	2.86	6.56	0.98	6.52
DTPAGe	-5.30	-1.04	3.16	5.93	0.07	0.36
DCzGe	-5.71	-1.27	3.30	6.35	0.30	2.19

DTPAGe   **DCzGe**

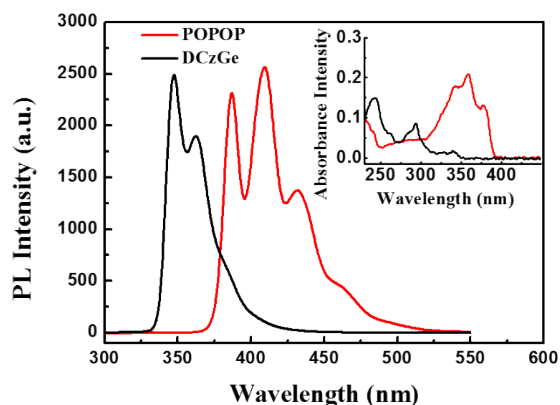**Fig. S1** Chemical structures of the designed molecules.

Fig. S2 Absorption and PL spectra of DCzGe and POPOP in cyclohexane used to measure the relative fluorescence quantum yield.
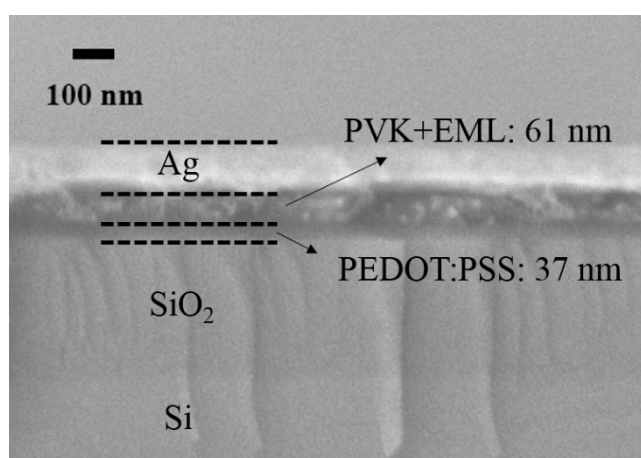

Fig. S3 SEM cross-section image of PVK/EML film on top of PEDOT:PSS-coated Si/SiO$_2$ slide. The organic layer was fabricated with the same method as used for device 5.
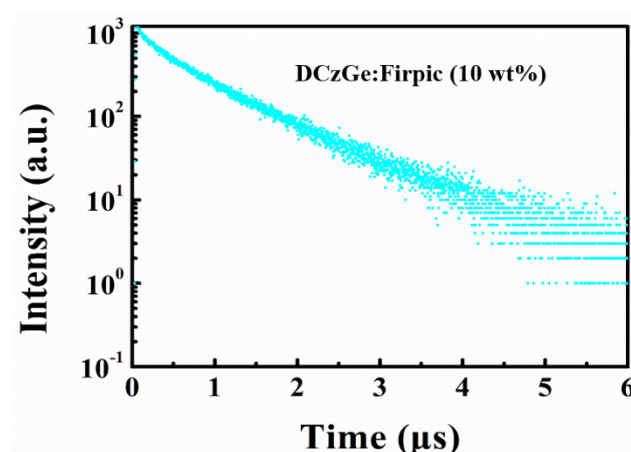

Fig. S4 The transient photoluminescence decay curve of 10 wt% FIrpic doped DCzGe thin film measured at 477 nm (at room temperature).

S1 K. S. Yook, S. E. Jang, S. O. Jeon and J. Y. Lee, *Adv. Mater.*, 2010, **22**, 4479.

S2 J. R. Lakowicz, *Principles of Fluorescence Spectroscopy, 2nd Ed.*, Kluwer Academic/Plenum Publishers, New York, London, Moscow, Dordrecht, 1999.

S3 A. M. Brouwer, *Pure Appl. Chem.*, 2011, **83**, 2213.

S4 C.-H. Hsieh, F.-I. Wu, C.-H. Fan, M.-J. Huang, K.-Y. Lu, P.-Y. Chou, Y.-H. O. Yang, S.-H. Wu, I. C. Chen, S.-H. Chou, K.-T. Wong and C.-H. Cheng, *Chem. -Eur. J.*, 2011, **17**, 9180.

S5 L. Hou, L. Duan, J. Qiao, W. Li, D. Zhang and Y. Qiu, *Appl. Phys. Lett.*, 2008, **92**, 263301.