Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Multiscale simulation of charge transport in a host material, *N,N'*-dicarbazole-3,5-benzene (mCP), for organic light-emitting diodes

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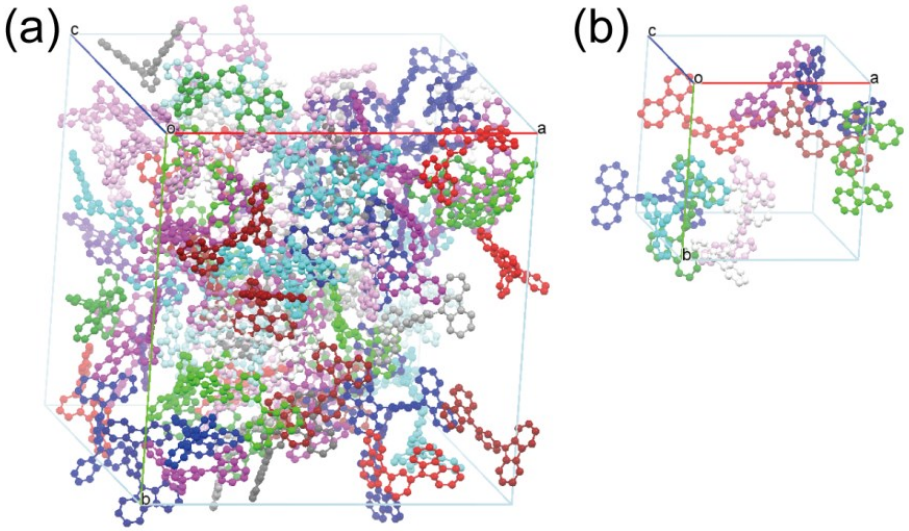
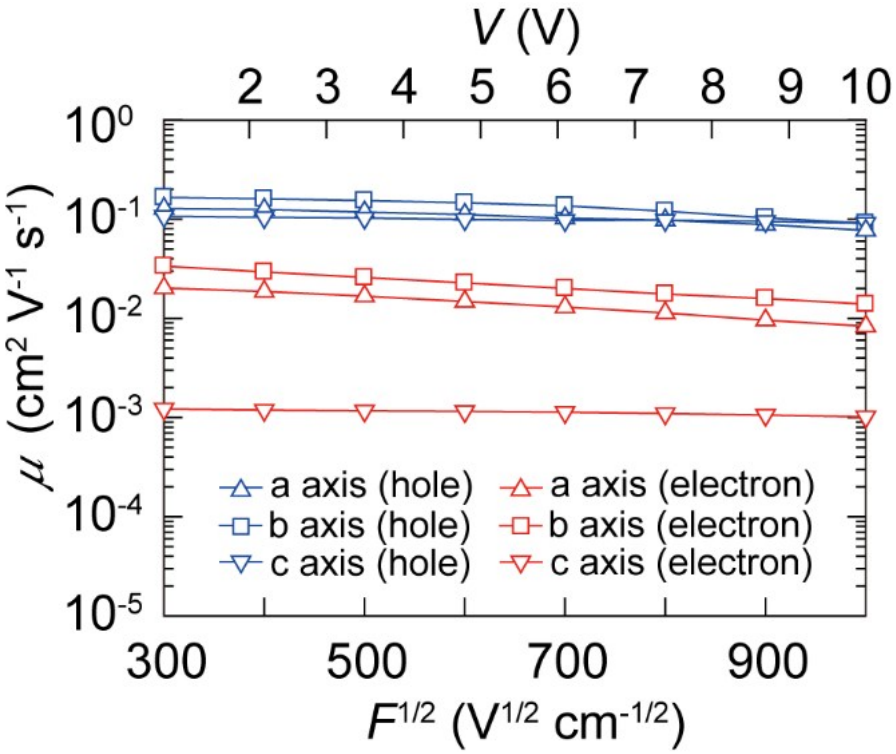
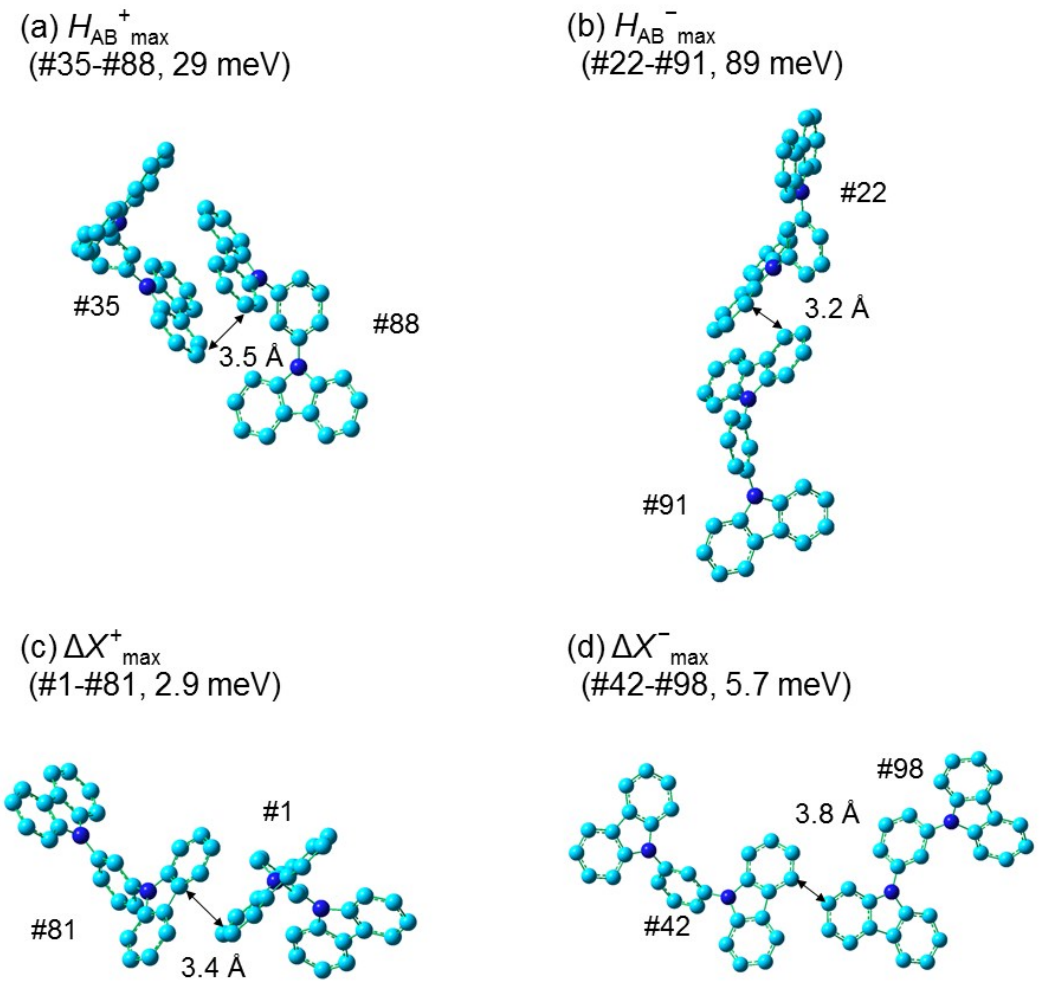


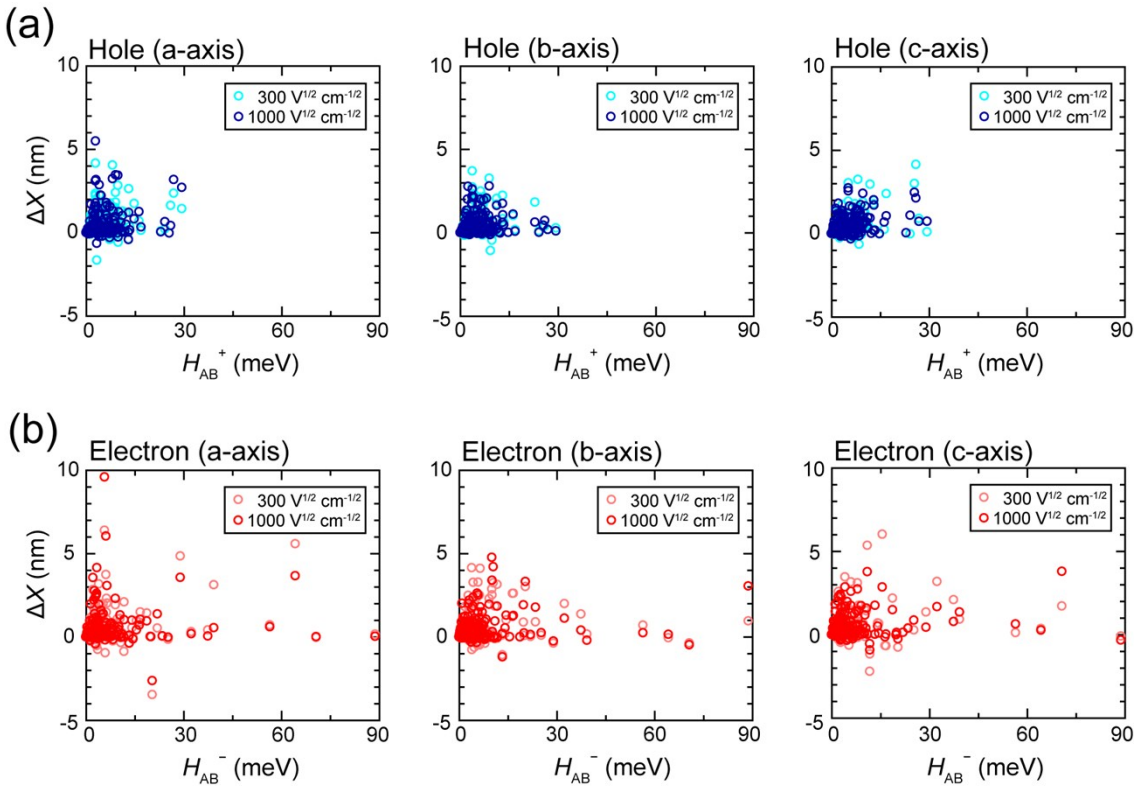
Supplementary Fig. S1: MD-constructed amorphous structures for (a) mCP-100 and (b) mCP-10. Each of the molecules is color-coded for clarity.



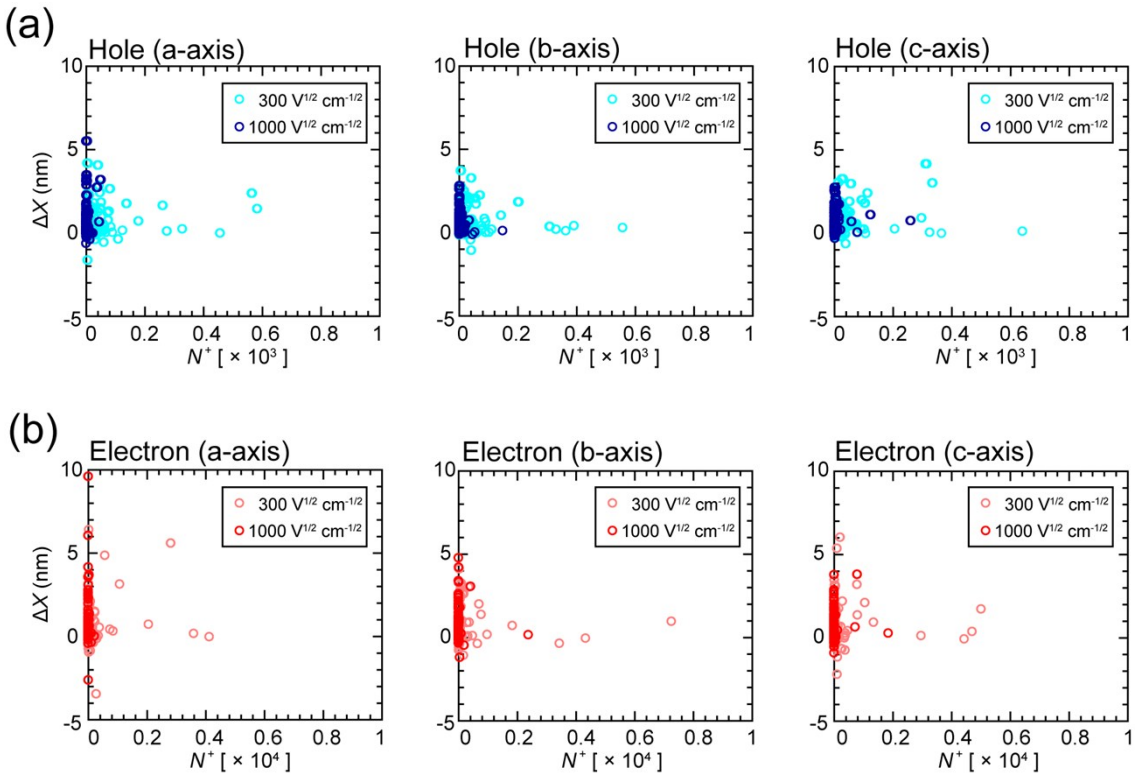
Supplementary Fig. S2: Simulated field depenence of the charge mobilities for the mCP-10 structure along the *a*-, *b*- and *c*-axes. The thickness was set to 100 nm.



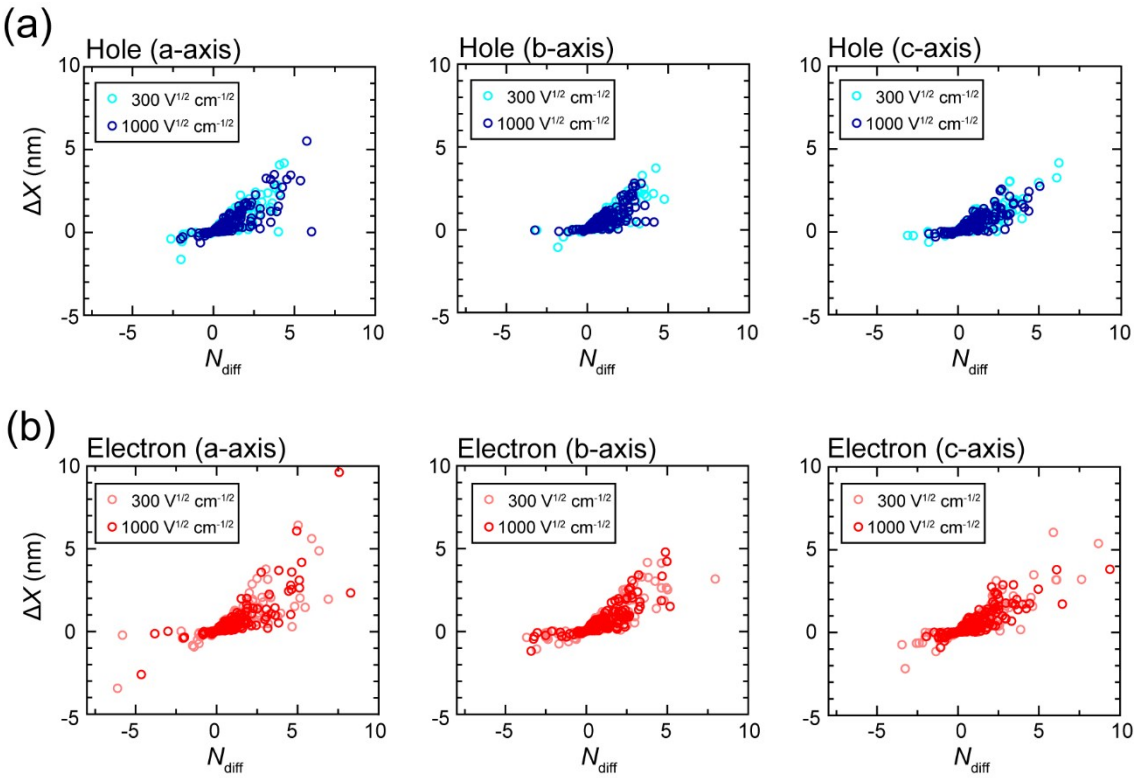
Supplementary Fig. S3: Pairs of molecules with the maximum values of H_{AB}^{+} and H_{AB}^{-} for (a) hole ($H_{AB}^{+}{}_{max}$) and (b) electron ($H_{AB}^{-}{}_{max}$), and pairs of molecules with the largest values of migration distance ΔX^{+} and ΔX^{-} for (c) hole ($\Delta X^{+}{}_{max}$) and (d) electron ($\Delta X^{-}{}_{max}$). The values are for 300 $V^{1/2}$ $cm^{-1/2}$ along the *a*-axis.



Supplementary Fig. S4: Correlation of H_{AB} and ΔX.



Supplementary Fig. S5: Correlation of N^+ and ΔX.

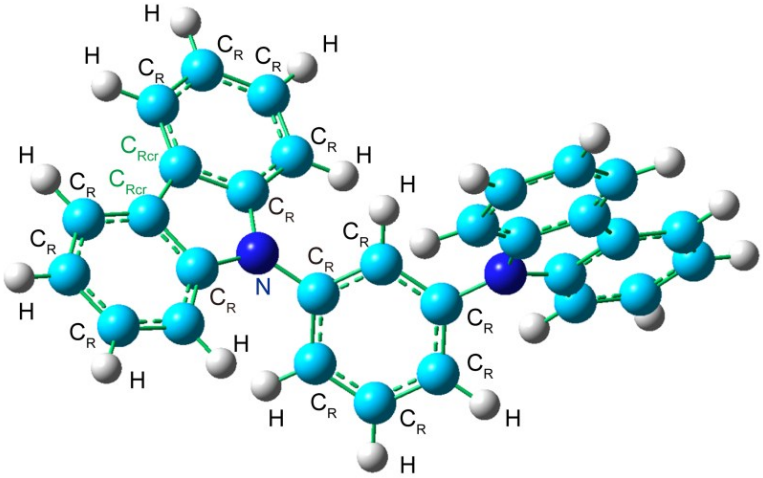


Supplementary Fig. S6: Correlation of N_{diff} and ΔX.

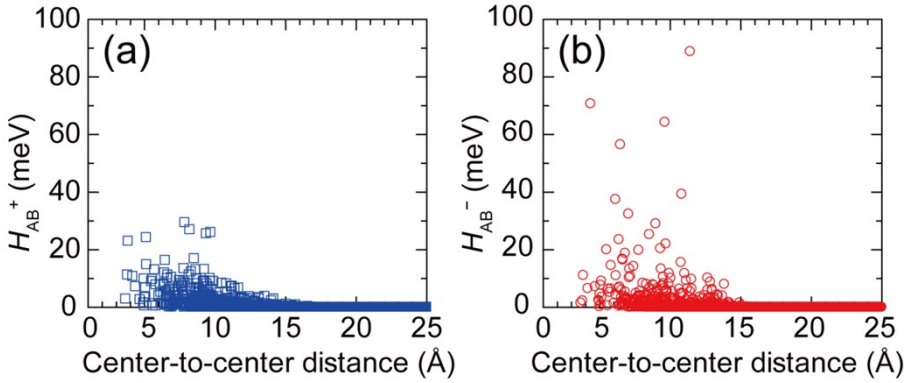
Calculation details

The Dreiding force field parameters were modified to keep the bond lengths and bond angles constant during the MD calculations, which are optimized at the DFT level (B3LYP/6-31G(d)). The manipulated parameters were as follows:

Bond stretch	$E = \frac{K_0}{2}(R - R_0)^2$	K_0 :$kcal\ mol^{-1}$Å^{-2} R_0 :Å
Angle bend	$E = \frac{K_0}{2}(\theta - \theta_0)^2$	K_0 :$kcal\ mol^{-1} degree^{-2}$ θ_0 :$degree$
Torsion	$E = \frac{1}{2}\sum_j \{B_j(1 - d_j cos[n_j\phi])\}$	B :$kcal\ mol^{-1}$ d : – n : –
Inversion	$E = K_0(1 - cos\omega_0)$	K_0 :$kcal\ mol^{-1}$ ω_0 :$degree$
Van der Waals	$E = D_0\left[\left(\frac{R_0}{R}\right)^{12} - 2\left(\frac{R_0}{R}\right)^6\right]$	
Coulombic	$E = C\frac{q_i q_j R_0}{\varepsilon R^2}$	C :Å $kcal\ mol^{-1} e^{-2}$ R_0 :Å
Hydrogen bond	$E = D_0\left[5\left(\frac{R_0}{R}\right)^{12} - 6\left(\frac{R_0}{R}\right)^{10}\right] cos^4\phi$	D_0 :$kcal\ mol^{-1}$ R_0 :Å



Supplementary Fig. S7: Structure and atom types of the mCP molecule.



Supplementary Fig. S8: Dependence of the electronic coupling (H_{AB}^{+} and H_{AB}^{-}) on the center-to-center distance (a) for holes and (b) for electrons, for mCP-100.

Supplementary Table S1: Manipulated force field parameters for the mCP molecule. The asterisks indicate the atoms of any type.

Parameter		R_0	θ_0	B	d	n	ω_0	K_0
Bond stretch	C_R-C_R	1.399						10500
	N- C_R	1.407						10500
	C_R-H	1.086						7000
	C_{Rcr}-C_{Rcr}	1.448						10500
	C_{Rcr}-C_R	1.399						10500
Angle bend	*- C_R-*		120					100
	- C_{Rcr}-		120					100
Torsion	*-C_R-C_R-*			25	1	2		
	-C_{Rcr}-C_{Rcr}-			25	1	2		
	-C_{Rcr}-C_R-			25	1	2		
Inversion	C_R-*-*-*-*						0	40
	C_{Rcr}-*-*-*-*						0	40

Supplementary Table S2: Manipulated force field parameters for the mCP molecule (non-bonded).

Parameter	R_0	D_0	C
Coulombic	1		332
Hydrogen bond	2.75	4	