Supporting Information For: The inherent mechanism of mechanochromism under different stress: electron cloud density distribution, J-type stacking, pore structure and collapse of J-type stacking

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Experimental
Measurement and characterization

\textsuperscript{1}H NMR spectra were obtained through a Varian inova-400-MHz NMR, the tetramethylsilane (TMS) was employed as the internal standard for calibration. \textsuperscript{19}F NMR spectra were obtained through a Varian inova-376-MHz NMR in CDCl\textsubscript{3} solvent. \textsuperscript{13}C NMR spectra were recorded on a Varian inova-100-MHz spectrometer and CDCl\textsubscript{3} was used as the solvent in all cases. The UV-vis absorption spectra were obtained from a spectrophotometer MaPada UV-3200PCS. Fluorescent emission spectra were obtained on a Hitachi F-2500 fluorescence spectrophotometer. Fluorescent quantum yields were acquired through a FLs980 full-featured Steady/Transient Fluorescence Spectrometer (Edinburgh). Glass transition temperature and melting point was measured by carried out DSC measurements using DSC Q2000 (TA, America). MALDI/HRMS were record on an UltrafleXtreme MALDI-TOF/TOF mass spectrometer (Bruker, Germany). Powder XRD measurements were performed on the D8 Advance (Bruker) with Cu K\textalpha radiation in the range of 10° < 2\theta < 90°. Digital photographs were taken by Canon 550D (Canon, Japan) digital cameras. Fluorescence lifetimes were measured by using an Edinburgh Instrument FLSP920 fluorescence spectrophotometer, and all the samples were excited at 360 nm. Fluorescence microscopy photos were obtained on OLYMPUS BX53. The theoretical calculation were calculated by density functional theory (DFT) in Gaussian 09 at the B3LYP/6-31G (d,p) level.

Materials and Synthesis.
THF and CH\textsubscript{2}Cl\textsubscript{2} were dried following the standardized procedures described previously. All the other chemicals and reagents used in this study were of analytical grade without further purification. In general, all the intermediates and final compounds were purified by column chromatography on silica gel (200-300 mesh), and crystallization from analytical grade solvents. Reactions were monitored by using thin layer chromatography (TLC). The synthetic routes for TPEDKB\textsubscript{2}O\textsubscript{Me}, TPEDKB\textsubscript{2}O\textsubscript{Et}, TPEDKB\textsubscript{2}OB\textsubscript{u}, TPEDKB\textsubscript{2}OH\textsubscript{e} and TPEDKB\textsubscript{2}ON\textsubscript{o} are shown in Scheme 1. Firstly, TPE was synthesized by using benzophenone as the reagent strictly follow the reported procedures; then Friedel-Crafts acylation reaction occurred between TPE and acetyl chloride, then the compound Ac-TPE are generated; Next, five \textbeta-diketonate intermediates and the corresponding complexes were prepared by condensation and boron-complexation reaction, respectively. The target molecules were characterized by \textsuperscript{1}H NMR, \textsuperscript{13}C NMR, \textsuperscript{19}F NMR, MALDI-TOF mass spectrometry thereafter.
2,2-difluoro-4-(4-methoxyphenyl)-6-(4-(1,2,2-triphenylvinyl)phenyl)-2H-1,3,2-dioxaborinin-1-ium-2-uide(TPEDKBF₂OHe)

NaH (60%, 0.20 g, 4.80 mmol) was added quickly to a dry flask which contains the solution of Methyl p-methoxybenzoate (0.48g, 2.88 mmol) in THF (20 mL) at room temperature. Then, acetyl-TPE (0.90 g, 2.40 mmol) was added later. After the mixture was refluxed under 90 °C for 24 h in argon atmosphere, it was cooled to room temperature. Then, the mixture was acidified with dilute HCl. The mixture was poured into water and extracted with dichloromethane for three times. Then the organic phase was combined and dried over anhydrous Na₂SO₄. The solvent was removed under reduced pressure and a yellow residue solid was collected. Then, the solid was dried under vacuum followed by dissolving in CH₂Cl₂ (50 mL). The boron trifluoride diethyl ether (0.6 mL, 4.80 mmol) was added to the above solution, which was stirred in argon environment with the pressure of 1 atm at room temperature for 24 h. In order to quench the reaction, water was added. The organic layer was separated and dried over Na₂SO₄. After removal of the solvent, the raw product was further purified by column chromatography (silica gel, petroleum ether/CH₂Cl₂, v/v = 2/1) to obtain the TPEDKBF₂OMe (0.53 g) as a yellow solid. Yield 40% m.p. 265.0–266.0 °C. ¹H NMR (400 MHz, CDCl₃) δ/ppm = 8.14 (d,J=12.0, 2H), 7.89 (d,J=8.0, 2H), 7.22-7.14 (m, 11H), 7.07-7.03 (m, 9H), 3.95 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): δ/ppm = 181.64, 180.89, 165.21, 161.77, 151.24, 143.58, 142.96, 142.92, 142.73, 139.54, 132.03, 131.49, 131.33, 131.31, 131.25, 129.93, 128.14, 128.04, 127.99, 127.76, 127.25, 126.98, 124.31, 114.64, 92.37, 55.79. ¹⁹F NMR (376 MHz, Chloroform-d) δ/ppm = -140.81 (d, J = 23.1 Hz). HRMS (MALDI-TOF): m/z 537.2046 [(M+H)⁺, calculated 537.2021].

4-(4-ethoxyphenyl)-2,2-difluoro-6-(4-(1,2,2-triphenylvinyl)phenyl)-2H-1,3,2-dioxaborinin-1-ium-2-uide(TPEDKBF₂OEt)

Compound TPEDKBF₂OEt was prepared by following the synthetic procedure for compound TPEDKBF₂OMe. The raw product was purified by column chromatography (silica gel, petroleum ether/CH₂Cl₂, v/v = 7/4), to afford TPEDKBF₂OEt (0.52 g) as a yellow solid. Yield: 38%. m.p. 286.0–287.0 °C. ¹H NMR (400 MHz, CDCl₃) δ/ppm = 8.13 (d,J=12.0, 2H), 7.88 (d,J=8.0, 2H), 7.22-7.214 (m, 11H), 7.07-7.00 (m, 9H), 4.18 (q,J=8.0, 2H), 1.49 (t,J=7.2, 3H). ¹³C NMR (100 MHz, CDCl₃): δ/ppm = 181.65, 180.75, 165.10, 151.17, 143.55, 142.97, 142.92, 142.74, 139.55, 132.01, 131.52, 131.33, 131.31, 131.25, 129.97, 128.11, 128.03, 127.99, 127.75, 127.24, 126.99, 126.97, 124.06, 115.03, 92.32 64.23, 14.59. ¹⁹F NMR (376 MHz, Chloroform-d) δ/ppm = -140.80 (d, J = 23.1 Hz). HRMS (MALDI-TOF): m/z 551.2197 [(M+H)⁺, calculated 551.2178].

4-(4-butoxyphenyl)-2,2-difluoro-6-(4-(1,2,2-triphenylvinyl)phenyl)-2H-1,3,2-dioxaborinin-1-ium-2-uide(TPEDKBF₂OBu)

Compound TPEDKBF₂OBu was synthesised by following the synthetic procedure for compound TPEDKBF₂OMe. The crude product was purified by column chromatography (silica gel, petroleum ether/CH₂Cl₂, v/v = 7/4), to afford TPEDKBF₂OBu (0.50 g) as a yellow solid. Yield: 35%. m.p. 287.0–289.0 °C. ¹H NMR (400 MHz, CDCl₃) δ/ppm = 8.12 (d,J=8.0, 2H), 7.88 (d,J=8.0, 2H), 7.22-7.14 (m, 11H), 7.07-7.01 (m, 9H), 4.10 (t,J=6.4, 2H), 1.87-1.80 (m, 2H), 1.59-1.49 (m, 2H), 1.02 (t,J=7.6, 3H). ¹³C NMR (100 MHz, CDCl₃): δ/ppm = 181.65, 180.73, 165.32, 159.49, 151.15, 143.54, 142.97, 142.92, 142.74, 139.56, 132.01, 131.52, 131.33, 131.31, 131.25, 129.98, 128.11, 128.03, 127.99, 127.75, 127.24, 126.97, 124.00, 115.05, 92.31, 68.38, 31.03, 19.16, 13.80. ¹⁹F NMR (376 MHz, Chloroform-d) δ/ppm = -140.82 (d, J = 23.1 Hz). HRMS (MALDI-TOF): m/z 579.2515 [(M+H)⁺, calculated 579.2491].

2,2-difluoro-4-(4-(hexyloxy)phenyl)-6-(4-(1,2,2-triphenylvinyl)phenyl)-2H-1,3,2-dioxaborinin-1-ium-2-uide(TPEDKBF₂OHe)

Compound TPEDKBF₂OHe was synthesised by following the synthetic procedure for compound TPEDKBF₂OMe. The crude product was purified by column chromatography (silica gel, petroleum ether/CH₂Cl₂, v/v = 7/4), to generated highly purified TPEDKBF₂OHe (0.53 g) as a yellow solid. Yield: 35%. m.p. 287.0–289.0 °C. ¹H NMR (400 MHz, CDCl₃) δ/ppm = 8.12 (d,J=8.0, 2H), 7.88 (d,J=8.0, 2H), 7.22-7.14 (m, 11H), 7.07-7.01 (m, 9H), 4.18 (t,J=6.4, 2H), 1.87-1.80 (m, 2H), 1.49 (q,J=8.0, 2H), 1.39-1.37 (m, 4H), 0.96-0.91 (m, 3H). ¹³C NMR (100 MHz, CDCl₃): δ/ppm = 181.65, 180.68, 165.33, 143.55, 142.93, 132.01, 131.53, 131.32, 131.25, 129.97, 128.12, 128.04, 127.99, 127.24, 127.00, 126.98, 92.33, 68.71, 31.52, 28.98, 25.62, 22.58, 14.03. ¹⁹F NMR (376 MHz, Chloroform-d) δ/ppm = -140.81 (d, J = 23.1 Hz). HRMS (MALDI-TOF): m/z 607.2931 [(M+H)⁺, calculated 607.2804].
2,2-difluoro-4-(4-(nonyloxy)phenyl)-6-(4-(1,2,2-triphenylvinyl)phenyl)-2H-1,3,2-dioxaborinin-1-ium-2-uide(TPEDKBF₂ONo)

Compound TPEDKBF₂ONo was synthesised by following the synthetic procedure for compound TPEDKBF₂OMe. The crude product was purified by column chromatography (silica gel, CH₂Cl₂–petroleum ether, v/v = 7/4), to produce highly purified TPEDKBF₂ONo (0.57 g) as a yellow solid. Yield: 36%. m.p. 287.0–289.0 °C. ¹H NMR (400 MHz, CDCl₃) δ/ppm = 8.12 (d, J=8.0, 2H), 7.88 (d, J=8.0, 2H), 7.22-7.14 (m, 11H), 7.07-7.00 (m, 9H), 4.09 (t, J=8.0, 2H), 1.88-1.81 (m, 2H), 1.51-1.32 (m, 12H), 0.91 (t, J=8.0, 3H); ¹³C NMR (100 MHz, CDCl₃): δ/ppm = 181.63, 180.65, 165.33, 164.95, 151.14, 143.54, 142.98, 142.75, 139.57, 132.01, 131.34, 131.32, 131.25, 131.23, 129.96, 128.12, 128.04, 127.99, 127.76, 126.98, 124.21, 123.96, 115.06, 114.96, 92.34, 68.71, 31.88, 29.51, 29.35, 29.26, 29.02, 25.95, 22.69, 14.52. ¹⁹F NMR (376 MHz, Chloroform-d) δ/ppm = -140.82 (d, J = 23.1 Hz). HRMS (MALDI-TOF): m/z 649.3406 [M-F]+, calculated 649.3273.

Table S1. HOMO/LUMO energy levels of TPEDKBF₂OMe, TPEDKBF₂OEt, TPEDKBF₂OBu, TPEDKBF₂OHe and TPEDKBF₂ONo.

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<th>Compound</th>
<th>gap (eV)</th>
<th>LUMO (eV)</th>
<th>HOMO (eV)</th>
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<td>TPEDKBF₂ONo</td>
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<td>-3.388</td>
<td>-5.018</td>
</tr>
</tbody>
</table>

Figure S1. Normalized UV-vis absorption and fluorescence emission spectra of TPEDKBF₂OMe (A), TPEDKBF₂OEt (B), TPEDKBF₂OBu (C), TPEDKBF₂OHe (D) and TPEDKBF₂ONo (E) in different solvents (1.0 x 10⁻⁵ mol/L), fluorescence were excited at 420nm.
Figure S2. Fluorescence spectra of TPEDKB2OEt (A), TPEDKB2OBu (B), TPEDKB2OHe (C) and TPEDKB2ONo (D) in THF and THF/water mixtures. Luminogen concentration: 1×10^{-5} mol/L; excitation wavelength: 420 nm.

Figure S3. Molecular conformation of TPEDKB2OMe in the crystal.
**Figure S4.** Molecular conformation of TPEDKBF$_2$OEt in the crystal.

**Figure S5.** Molecular conformation of TPEDKBF$_2$OBu in the crystal.

**Figure S6.** Molecular conformation of TPEDKBF$_2$OHe in the crystal.
Figure S7. Molecular conformation of TPEDKBF$_2$ONO in the crystal.

Figure S8 $^1$H NMR (400 MHz) spectrum of compound TPEDKBF$_2$OMe in CDCl$_3$. 
Figure S9 $^{13}$C NMR (100 MHz) spectrum of compound TPEDKBF$_2$OMe in CDCl$_3$.

*19F NMR (376 MHz) spectrum of compound TPEDKBF$_2$OMe in CDCl$_3$.*
Figure S11 $^1$H NMR (400 MHz) spectrum of compound TPEDKBF$_2$OEt in CDCl$_3$.

Figure S12 $^{13}$C NMR (100 MHz) spectrum of compound TPEDKBF$_2$OEt in CDCl$_3$. 
Figure S13 $^{19}$F NMR (376 MHz) spectrum of compound TPEDKB$_2$OEt in CDCl$_3$.

Figure S14 $^1$H NMR (400 MHz) spectrum of compound TPEDKB$_2$OBu in CDCl$_3$. 
Figure S15 $^{13}$C NMR (100 MHz) spectrum of compound TPEDKBF$_2$OBu in CDCl$_3$.

Figure S16 $^{19}$F NMR (376 MHz) spectrum of compound TPEDKBF$_2$OBu in CDCl$_3$. 
Figure S17 $^1$H NMR (400 MHz) spectrum of compound TPEDKBF$_2$OHe in CDCl$_3$.

Figure S18 $^{13}$C NMR (100 MHz) spectrum of compound TPEDKBF$_2$OHe in CDCl$_3$. 
Figure S19 $^{19}$F NMR (376 MHz) spectrum of compound TPEDKBF$_2$OHe in CDCl$_3$.

Figure S20 $^1$H NMR (400 MHz) spectrum of compound TPEDKBF$_2$ONo in CDCl$_3$. 
Figure S21 $^{13}$C NMR (100 MHz) spectrum of compound TPEDKB$\text{F}_2\text{ONo}$ in CDCl$_3$. 

$^{19}$F NMR (376 MHz; Chloroform-d$_3$): $-40.92$ (d, $J_F^F = 23.1$ Hz).
Figure S22 $^{19}$F NMR (376 MHz) spectrum of compound TPEDKBF$_2$ONo in CDCl$_3$.

Figure S23 MALDI/TOF MS spectrum of compound TPEDKBF$_2$OMe.

Figure S24 MALDI/TOF MS spectrum of compound TPEDKBF$_2$OEt.
**Figure S25** MALDI/TOF MS spectrum of compound **TPEDKBF₂OBu**.

**Figure S26** MALDI/TOF MS spectrum of compound **TPEDKBF₂OHe**.
Figure S27 MALDI/TOF MS spectrum of compound TPEDKBF$_2$ONo.