Supporting Information

Breakdown of Interference Rules in Azulene, a Non-Alternant Hydrocarbon

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![Additional Figures](image-url)

**Figure S1:** Two-dimensional conductance vs displacement histograms for 1,3Az; 2,6Az; 4,7Az; and 5,7Az. Histograms were constructed by aligning each individual conductance vs displacement trace at the end of the 1G₀ plateau and then overlaying all traces. Dashed lines indicate the step-lengths obtained from the 2D histograms. Step-lengths are computed by integrating all counts in the conductance feature, and creating a 1D line profile. The step-length is then obtained by finding where the line profile falls to 20% of its peak value.
**Figure S2:** (a) One-dimensional, logarithmically binned conductance histogram, and (b) 2-dimensional conductance vs. displacement histogram for 1,3PyAz. We find that 1,3PyAz has a calculated length of 1.03nm (structure optimized using density functional theory, B3LYP/6-31G*), a 2D histogram step length of 0.56nm, and a most probable conductance of $9 \times 10^{-5} G_0$ (from log-binned histogram). The dashed line indicates the measured step-length as determined by the method described in the caption of Figure S1.

**Figure S3:** UV-vis spectra of pyridine-linked azulene molecule along with the four methyl-sulfide linked derivatives. Inset: magnification of the region between 400 and 800 nm ($S_0$-$S_1$ transition). All solutions are at a concentration of 10µM.
2) Theoretical methods:

We use a model molecular system with the azulene and naphthalene backbone connected to linkers consisting of an ethynyl group for the calculations carried out here. We minimize the geometry for these model systems using density functional theory. We then describe exchange and correlation effects in the GW approximation, attach the molecules to featureless, wideband leads and calculate the transmission using the Landauer-Büttiker formula. More details about the GW method can be found in the work of Thygesen and Rubio, but in brief we represent all Green’s functions and self-energies on a energy grid on the real axis and perform a self-consistent calculation for a central region coupled to non-interacting leads. We use an energy grid extending from -100eV to 100eV with a grid spacing of 0.0025eV and a numerical value for the imaginary “infinitesimal” used in the retarded Green’s function of twice the energy grid spacing (0.005eV). For these calculations, we only consider the π system of the molecule which is modeled using a Hamiltonian of the Pariser-Parr-Pople (PPP) type consisting of a simple nearest neighbor tight-binding part \( h = t \sum_{<ij>,\sigma} c_{i\sigma}^+ c_{j\sigma} \) and a part describing the electron-electron interactions \( V_{int} = \sum_i V_{ii} n_i n_i + \frac{1}{2} \sum_{i \neq j} V_{ij} (n_i - 1)(n_j - 1) \), where \( c_{i\sigma}^+ \) (\( c_{i\sigma} \)) creates (annihilates) an electron with spin \( \sigma \) in a \( p_z \) orbital on the \( i \) th atom and \( n_i = \sum_{\sigma} c_{i\sigma}^+ c_{i\sigma} \). For simplicity, we use a distance independent hopping parameter of \( t = -2.5eV \) and Ohno’s parameterization for the interactions described by an onsite repulsion \( U = 10eV \) (\( V_{ij} = U / \sqrt{1 + 0.6117 r_{ij}^2} \), where \( r_{ij} \) is distance between atom \( i \) and \( j \) in Angstrom). The onsite energy of the \( p_z \) orbitals is set to zero. We mention that despite the simplicity of the PPP Hamiltonian, the trends in the experimentally measured optical excitations for azulene and naphthalene are well captured. We have diagonalized the Hamiltonian for the molecules in gas phase (without linkers) exactly, which for azulene yields an \( S_0-S_1 \) and \( S_0-S_2 \) excitation energy of 1.6eV and 3.1eV. The calculated charge excitation gap of azulene is 6.4eV. For naphthalene we find a considerably larger \( S_0-S_1 \) excitation energy of 3.9eV while the charge excitation gap is 8.2eV. This is in good qualitative agreement with experiments considering that the linker groups were not included. Further, the trend in the shift of the excitation energy with substitution pattern
using a simple 2-atom linker is captured. We therefore believe that the PPP Hamiltonian captures the essential features of the naphthalene and azulene molecules.

![Transmission spectra for an azulene without linkers attached to wide-band electrodes at different points as indicated. The tight-binding model treats each atom with an on-site energy, $\varepsilon$, and is coupled to its nearest neighbors by an energy $\tau$. Linking atoms are coupled to leads using an imaginary self-energy, $-i\Gamma/2$. The parameters used for this calculations are: on-site energy $\varepsilon=0$, inter-atom coupling $\tau=4$ and electrode coupling $\Gamma=-3$.]

**Figure S4:** Transmission spectra for an azulene without linkers attached to wide-band electrodes at different points as indicated. The tight-binding model treats each atom with an on-site energy, $\varepsilon$, and is coupled to its nearest neighbors by an energy $\tau$. Linking atoms are coupled to leads using an imaginary self-energy, $-i\Gamma/2$. The parameters used for this calculations are: on-site energy $\varepsilon=0$, inter-atom coupling $\tau=4$ and electrode coupling $\Gamma=-3$.

3) **Synthetic Methods**

**General Methods:**

Chemicals were purchased from Sigma-Aldrich and used as received, unless otherwise noted. All reactions were performed in oven-dried round bottom flasks, unless otherwise noted. $^1$H and $^{13}$C nuclear magnetic resonance spectra were recorded at 300 K on a Bruker DRX300 (300MHz) or Bruker DRX400 (400MHz) FT NMR spectrometer. High-resolution mass spectra were from a JMS-HX110 HF mass spectrometer (ionization mode: FAB+). Uv-vis absorption spectra were taken on a Shimadzu UV-1800 spectrophotometer.
**Synthetic Procedures:**

6-bromo-4, 4-dimethylthiochroman,\(^6\) 2, 5-dimethyl-3-bromothiophene-S, S-dioxide \(^3\,^7,^8\) 1, 3-dibromoazulene,\(^9\) 4, 7-dibromoazulene\(^10\) and 2,4-Dibromo-3-methylthiophene (10)\(^11\) were prepared as reported.

To a stirred solution of 6-bromo-4,4-dimethylthiochroman \(^{11}\) (2.0g, 7.8mmol) in 40ml dry THF was slowly added 2.3M n-BuLi (3.7ml, 8.6mmol) at -78°C under Ar. The resulting mixture was stirred at the same temperature for another hour, and then PinBop (3.2ml, 15.6mmol) was added via syringe. The reaction flask was allowed to warm up to room temperature and left to stir overnight. The mixture was quenched with methanol and water (40ml); then it was extracted with dichloromethane (3 x 50ml). The combined organic solvents were washed with brine, dried over Mg\(_2\)SO\(_4\). After removing the solvent, the residue was purified by flash chromatography (ethyl acetate/hexane = 1:10) to give a yellowish white solid 2 (2g, 84% yield). \(^1\)H NMR (400MHz, CDCl\(_3\), ppm): \(\delta 7.77 (d, J = 0.8 \text{ Hz}, 1H), 7.45 (dd, J = 8.0, 1.2 \text{ Hz}, 1H), 7.09 (d, J = 8.0 \text{ Hz}, 1H), 3.03 (m, 2H), 1.95 (m, 2H), 1.35 (s, 6H), 1.33 (s, 12H).\(^\text{13}\)C NMR (100MHz, CDCl\(_3\), ppm): \(\delta 141.2, 136.2, 132.7, 132.2, 126.0, 83.6, 37.7, 32.9, 30.1, 24.9, 23.3.\) HR-MS (FAB) \(m/z\) calcd for C\(_{17}\)H\(_{25}\)O\(_2\)SB: 304.1672, found: 304.1676.
2, 5-dimethyl-3-bromothiophene-5, 5-dioxide 3\textsuperscript{7,8} (1.72 g, 7.71 mmol) was dissolved in 150 mL dichloromethane under argon. The solution was cooled down to 0 °C, then a solution of dimethylaminofulvene 4 (9.33 g, 7.71 mmol) in 12 mL dichloromethane was added over a period of 1 hour. The mixture was stirred at 0 °C for 6 h before the addition of another 0.5 equivalents of dimethylaminofulvene 4 (dissolved in 5 mL dichloromethane). Then the reaction mixture was warmed up to room temperature and stirred over night. Water (50 mL) was added, the mixture was extracted with dichloromethane (3 × 30 mL), the combined organic phases was washed with water (3 × 50 mL) and dried with sodium sulfate. After removing the solvent, the crude product was purified by chromatography (ethyl acetate/hexane = 1:10) using alumina to give 4,7-dimethyl-6-bromoazulene 5 as a dark solid (692 mg, yield: 38%). \textsuperscript{1}H NMR (400 MHz, CDCl\textsubscript{3}, ppm): \(\delta\) 8.30 (s, 1H), 7.82 (t, \(J = 3.6\) Hz, 1H), 7.75 (s, 1H), 7.31 (d, \(J = 3.6\) Hz, 1H), 7.26 (d, \(J = 4.4\) Hz, 1H), 2.83 (s, 3H), 2.75 (s, 3H). \textsuperscript{13}C NMR (100 MHz, CDCl\textsubscript{3}, ppm): \(\delta\) 142.6, 138.6, 137.1, 136.3, 136.0, 135.2, 130.1, 130.0, 119.3, 116.1, 30.3, 24.1. HR-MS (FAB) m/z calcd for C\textsubscript{12}H\textsubscript{11}Br: 235.1237, Found (isotopic pattern): 234.0044, 235.1237, 236.0022.
4,7-dimethyl-6-bromoazulene 5 (235 mg, 1 mmol), compound 2 (335 mg, 1.1 mmol), Pd(PPh$_3$)$_2$Cl$_2$ (70 mg, 0.1 mmol) and K$_2$CO$_3$ (276 mg, 2 mmol) were charged in a 25 mL Schlenk flask under argon, then 11 mL degassed THF/H$_2$O (10:1) was added. The result mixture was heated to 70 °C and stirred for 24 h. After cooled down to room temperature, water (10 mL) was added, the reaction mixture was extracted with dichloromethane (3 × 10 mL), the combined organic phase was washed with water (3 × 15 mL) and dried over sodium sulfate. After removing the solvent under reduced pressure, the crude mixture was purified by silica column chromatography (ethyl acetate/hexane = 1:10) to give compound 6 as a dark blue solid (284 mg, 84%). $^1$H NMR (400 MHz, CDCl$_3$, ppm): δ 8.40 (s, 1H), 7.82 (d, $^J_1 = 4$ Hz, 1H), 7.31-7.34 (m, 2H), 7.29 (d, $^J_1 = 4$ Hz, 1H), 7.15-7.19 (m, 2H), 7.02 (d, $^J_1 = 8$ Hz, 1H), 3.10 (t, $^J_1 = 6$ Hz, 2H), 2.39 (s, 3H), 2.88 (s, 3H), 2.04 (t, $^J_1 = 6$ Hz, 2H), 1.38 (s, 6H). $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): δ 150.3, 143.4, 142.2, 141.7, 139.8, 139.0, 135.9, 135.3, 130.5, 128.9, 128.7, 126.7, 126.3, 125.9, 118.0, 114.6, 37.7, 33.1, 30.3, 26.1, 24.6, 23.1. HR-MS (FAB) m/z calcd for C$_{23}$H$_{24}$S: 332.1599, Found: 332.1607.

Compound 6 (200 mg, 0.6 mmol), Bis(pinacolato)diboron (B$_2$Pin$_2$, 76 mg, 0.3 mmol), [Ir(OMe)(Cod)]$_2$ (20 mg, 0.03 mmol) and 4,4’-di-tert-butyl-2,2’-bipyridyl (dtbpy, 32 mg, 0.12
mmol) were charged in a 25-mL reaction vial under argon, then 10 mL of cyclohexane was added. The resulting mixture was heated to 90 °C and stirred for 24 h. After cooled down to room temperature, the solvent was removed under reduced pressure, and the dark residue was purified by silica column chromatography (ethyl acetate/hexane = 1:10) to give compound 7 as a purple solid (94 mg, 34%). $^1$H NMR (400 MHz, CDCl$_3$, ppm): δ 8.35 (s, 1H), 7.66 (s, 1H), 7.63 (s, 1H), 7.28 (d, $J = 2$ Hz, 1H), 7.15 (d, $J = 8$ Hz, 1H), 7.06 (s, 1H), 6.97 (dd, $J_1 = 6.4$, 2 Hz, 1H), 3.08 (t, $J = 6$ Hz, 2H), 2.85 (s, 3H), 2.33 (s, 3H), 2.02 (t, $J = 6$ Hz, 2H), 1.42 (s, 12H), 1.35 (s, 6H). $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): δ 151.9, 145.3, 142.2, 141.7, 141.4, 139.6, 136.3, 130.6, 128.8, 128.7, 126.6, 126.3, 125.8, 121.2, 83.6, 37.7, 33.1, 30.3, 29.7, 26.1, 24.9, 24.7, 23.1. HR-MS (FAB) m/z calcd for C$_{29}$H$_{35}$BO$_2$: 458.2451, Found: 458.2456.

![2,6-Azulene](image)

Compound 7 (90 mg, 0.2 mmol), compound 1 (51 mg, 0.2 mmol), Pd(PPh$_3$)$_2$Cl$_2$ (14 mg, 0.02 mmol) and K$_2$CO$_3$ (55 mg, 0.4 mmol) were charged 25-mL reaction vial under argon, then 3.5 mL degassed THF/H$_2$O (6:1) was added. The result mixture was heated to 70 °C and stirred for 24 h. After cooled down to room temperature, the solvent was removed under reduced pressure, and the dark residue was purified by silica column chromatography (ethyl acetate/hexane = 1:10) to give compound **2,6-Azulene** as a yellow-blue solid (80 mg, 80%). $^1$H NMR (400 MHz, CDCl$_3$, ppm): δ 8.28 (s, 1H), 7.98 (d, $J = 2$ Hz, 1H), 7.67 (dd, $J_1 = 6.4$ Hz, $J_2 = 2$ Hz, 1H), 7.53 (d, $J = 2$ Hz, 1H), 7.49 (d, $J = 2$ Hz, 1H), 7.31 (d, $J = 2$ Hz, 1H), 7.15-7.20 (m, 2H), 7.11 (s, 1H), 7.01 (dd, $J_1 = 6$, 2 Hz, 1H), 3.09 (m, 4H), 2.88 (s, 3H), 2.36 (s, 3H), 2.04 (m, 4H), 1.46 (s, 6H), 1.37 (s, 6H). $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): δ 149.1, 148.3, 142.3, 142.2, 142.1, 141.7, 140.2, 138.6, 137.2, 132.8, 132.0, 130.4, 129.8, 129.6, 127.0, 126.8, 126.2, 126.0, 125.3, 125.1, 113.7, 111.0, 37.8, 37.7, 33.1, 30.3, 30.2, 26.2, 24.6, 23.2, 23.1. HR-MS (FAB) m/z calcd for C$_{34}$H$_{36}$S$_2$: 508.2258, Found: 508.2265.
1,3-dibromoazulene $8^9$ (33 mg, 0.12 mmol), compound $2$ (140 mg, 0.46 mmol), Pd(PPh$_3$)$_2$Cl$_2$ (4 mg, 0.006 mmol) and K$_2$CO$_3$ (64 mg, 0.46 mmol) were charged in a 10 ml 2-neck round bottom flask under argon, and then 3 ml of degassed THF/H$_2$O (4/1) was added via a syringe. The reaction was heated at 70°C for 7 hr and then cooled down to room temperature. Water (10 ml) was added, the resulting green solution was extracted with dichloromethane (10 ml x 3). The combined organic solvents were washed with brine and dried over MgSO$_4$. After removing solvents, the residue was purified by flash chromatography (hexane/dichloromethane=2:1) to give **1,3-Azulene** as a green solid (41 mg, 74%). $^1$H NMR (400 MHz, CDCl$_3$, ppm): $\delta$ 8.46 (d, $J = 9.6$ Hz, 2H), 8.04 (s, 1H), 7.62 (d, $J = 1.6$ Hz, 2H), 7.55 (t, $J = 10$ Hz, 1H), 7.33 (dd, $J = 8.0$, 1.6 Hz, 2H), 7.22 (d, $J = 8.0$ Hz, 2H), 7.08 (t, $J = 10$ Hz, 2H), 3.10 (m, 4H), 2.05 (m, 4H), 1.41 (s, 12H). $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): $\delta$ 142.4, 139.1, 136.8, 136.6, 136.3, 133.1, 130.7, 130.3, 128.3, 127.6, 127.0, 123.4, 38.0, 33.4, 30.5, 23.4. HR-MS m/z calcd for C$_{32}$H$_{32}$S$_2$: 480.1945, found: 480.1935.

4,7-dibromoazulene $9^{10}$ (25 mg, 0.09 mmol), compound $2$ (106 mg, 0.36 mmol), Pd(PPh$_3$)$_2$Cl$_2$ (3 mg, 0.004 mmol) and K$_2$CO$_3$ (50 mg, 0.36 mmol) were charged in a 10 ml 2-neck round bottom flask under argon, and then 3 ml of degassed THF/H$_2$O (4/1) was added via a syringe. The reaction was heated at 70°C for 4 hr and then cooled down to room temperature. Water (10 ml) was added, the resulting blue solution was extracted with DCM (10 ml x 3). The combined
organic solvents were washed with brine and dried over MgSO₄. After removing solvents, the residue was purified by flash chromatography (hexane/dichloromethane=2:1) to give 4, 7-Azulene as a blue solid (35mg, 85%). $^1$H NMR (400MHz, CDCl₃, ppm): δ 8.63 (d, J = 1.6 Hz, 1H), 7.86 (t, J = 3.6 Hz, 1H), 7.82 (dd, J = 10.8, 2.0 Hz, 1H), 7.68 (d, J = 2.0 Hz, 1H), 7.64 (d, J = 2.0 Hz, 1H), 7.49 (d, J = 3.6 Hz, 1H), 7.35 (dt, J = 8.0, 2.0 Hz, 2H), 7.24 (s, 1H), 7.22 (d, J = 1.6 Hz, 1H), 7.20 (s, 1H), 3.10 (m, 4H), 2.04 (m, 4H), 1.43 (s, 6H), 1.39 (s, 6H). $^{13}$C NMR (100MHz, CDCl₃, ppm): δ 149.3, 142.6, 140.6, 137.7, 136.9, 136.3, 128.0, 127.2, 126.5, 126.4, 125.9, 125.6, 120.4, 118.5, 37.9, 33.4, 33.3, 30.5, 23.4, 23.3. HR-MS m/z calcd for C₃₂H₃₂S₂: 480.1945, found: 480.1948.

Scheme S2. Synthetic route of 5,7-Azulene.

2,4-Dibromo-3-methylthiophene 10 (942 mg, 3.68 mmol) was dissolved in 15 mL CH₂Cl₂ and cooled down to 0 °C, HOF•CH₃CN solution (0.23 M) was slowly added to the reaction mixture and the reaction was stopped after 2h by adding a saturated solution of NaHCO₃. The organic material was extracted with CH₂Cl₂, washed with water and dried over Na₂SO₄. The crude product was purified by recrystallization from hot hexanes to afford 2,4-Dibromo-3-methylthiophene-S, S-dioxide (11) as a white solid (310 mg, yield: 29%). $^1$H NMR (400 MHz, CDCl₃, ppm): 7.01 (s, 1H), 2.12 (s, 3H). $^{13}$C NMR (100 MHz, CDCl₃, ppm): δ 136.7, 131.1, 128.7, 118.4, 15.5. HR-MS (FAB) m/z calcd for C₅₂H₃₂Br₂O₂S: 888.9675, Found: 888.9651.
2,4-Dibromo-3-methylthiophene-S, S-dioxide 11 (310 mg, 1.07 mmol) was dissolved in 15 mL dichloromethane under argon. The solution was cooled down to 0 °C, then a solution of dimethylaminofulvene 4 (130 mg, 1.07 mmol) in 2 mL dichloromethane was added over a period of 30 min. The mixture was stirred at 0 °C for 6 h before the addition of another 0.5 equivalent of dimethylaminofulvene (dissolved in 2 mL dichloromethane). Then the reaction mixture was warmed up to room temperature and stirred overnight. After removing the solvent, the crude product was purified by chromatography (hexanes) using alumina to give 5,7-Dibromo-6-methylazulene 12 as a blue solid (36 mg, yield: 11%). $^1$H NMR (400 MHz, CDCl$_3$, ppm): 8.80 (s, 2H), 7.88 (t, $J = 4$ Hz, 1H), 7.32 (d, $J = 4$ Hz, 2H), 3.08 (s, 3H). $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): δ 145.1, 139.6, 139.4, 136.3, 120.2, 119.0, 35.9. HR-MS (FAB) m/z calcd for C$_{11}$H$_8$Br$_2$: 299.9925, Found: 299.8973.

5,7-Dibromo-6-methylazulene 12 (35 mg, 0.117 mmol), compound 2 (89 mg, 0.292 mmol), Pd(PPh$_3$)$_2$Cl$_2$ (8 mg, 0.011 mmol) and K$_2$CO$_3$ (65 mg, 0.47 mmol) were charged in a reaction vial under argon, then 2.1 mL degassed THF/H$_2$O (20:1) was added. The result mixture was heated to 70 °C and stirred for 24 h. After cooled down to room temperature, the solvent was removed under high vacuum, and the crude mixture was purified by chromatography (dichloromethane/hexanes = 1:3) to give 5,7-Azulene as a dark blue solid (45 mg, 78 %). $^1$H NMR (400 MHz, CDCl$_3$, ppm): 8.34 (s, 2H), 7.86 (t, $J = 3.6$ Hz, 1H), 7.36 (d, $J = 1.2$ Hz, 2 H), 7.29 (d, $J = 3.6$ Hz, 2H), 7.16 (d, $J = 8.4$ Hz, 2H), 7.06 (dd, $J = 1.6$ Hz, 2H), 3.07-3.10 (m, 4H), 2.12 (s, 3H), 2.01-2.04 (m, 4H), 1.37 (s, 12H). $^{13}$C NMR (100 MHz, CDCl$_3$, ppm): δ 145.3, 142.7, 142.0, 138.2, 137.8, 137.2, 137.0, 129.9, 127.4, 126.8, 126.4, 117.7, 37.9, 32.9, 30.4, 27.8, 23.1. HR-MS (FAB) m/z calcd for C$_{33}$H$_{34}$S$_2$: 494.7650, Found: 494.7642.
1,3-dibromoazulene 8 (100 mg, 0.35 mmol), Pyridine-4-boronic acid 13 (90%, 172 mg, 1.4 mmol), Pd(PPh₃)₂Cl₂ (12 mg, 0.017 mmol) and K₂CO₃ (193 mg, 1.4 mmol) were charged in a 20-mL reaction vial under argon, and then 6 ml of degassed THF/H₂O (5/1) was added via a syringe. The reaction was heated at 70°C for overnight and then cooled down to room temperature. Water (10 ml) was added, the resulting green solution was extracted with dichloromethane (10ml x 3). The combined organic solvents were washed with brine and dried over Na₂SO₄. After removing solvents, the residue was purified by flash chromatography (hexane/dichloromethane=2:1) to give 1, 3-Py-Azulene as a green solid (50 mg, 50%) ¹H NMR (400MHz, CDCl₃, ppm): δ 7.34 (t, J = 10 Hz, 2H), 7.56 (m, 4H), 7.76 (t, J = 10 Hz, 1H), 8.19 (s, 1H), 8.65 (d, J = 9.6 Hz, 2H), 8.73 (m, 4H). ¹³C NMR (100 MHz, CDCl₃, ppm): δ 124.07, 125.55, 127.54, 136.14, 136.74, 137.70, 139.91, 144.14, 149.96.

4) References:
5) NMR Spectra