Supporting Information for Size- and Voltage-Dependent Electron Transport of C_2N-Rings-Based Molecular Chains

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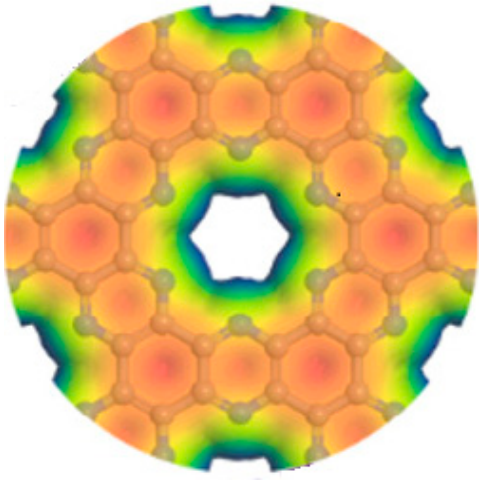

Figure S1 Molecular electrostatic potential for the pore (unit cell) of C_2N monolayer [17].

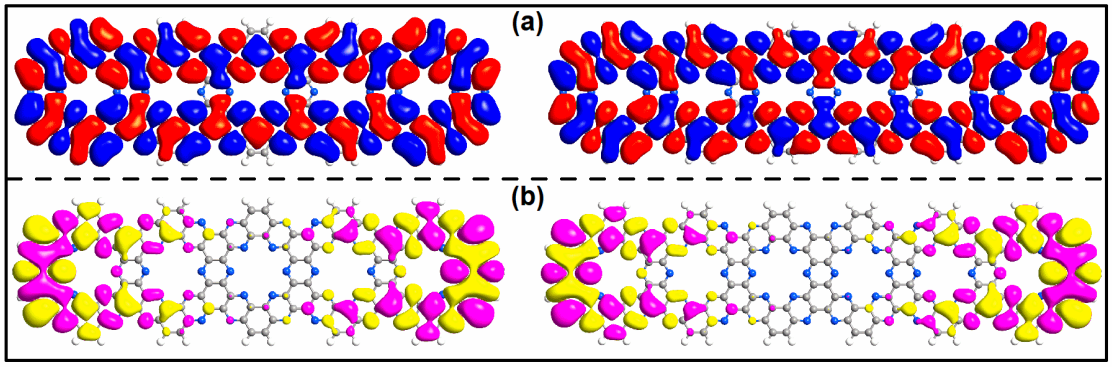

Figure S2 (a-b) LUMOs and HOMOs of Device C_2N ring5 and 6, respectively.

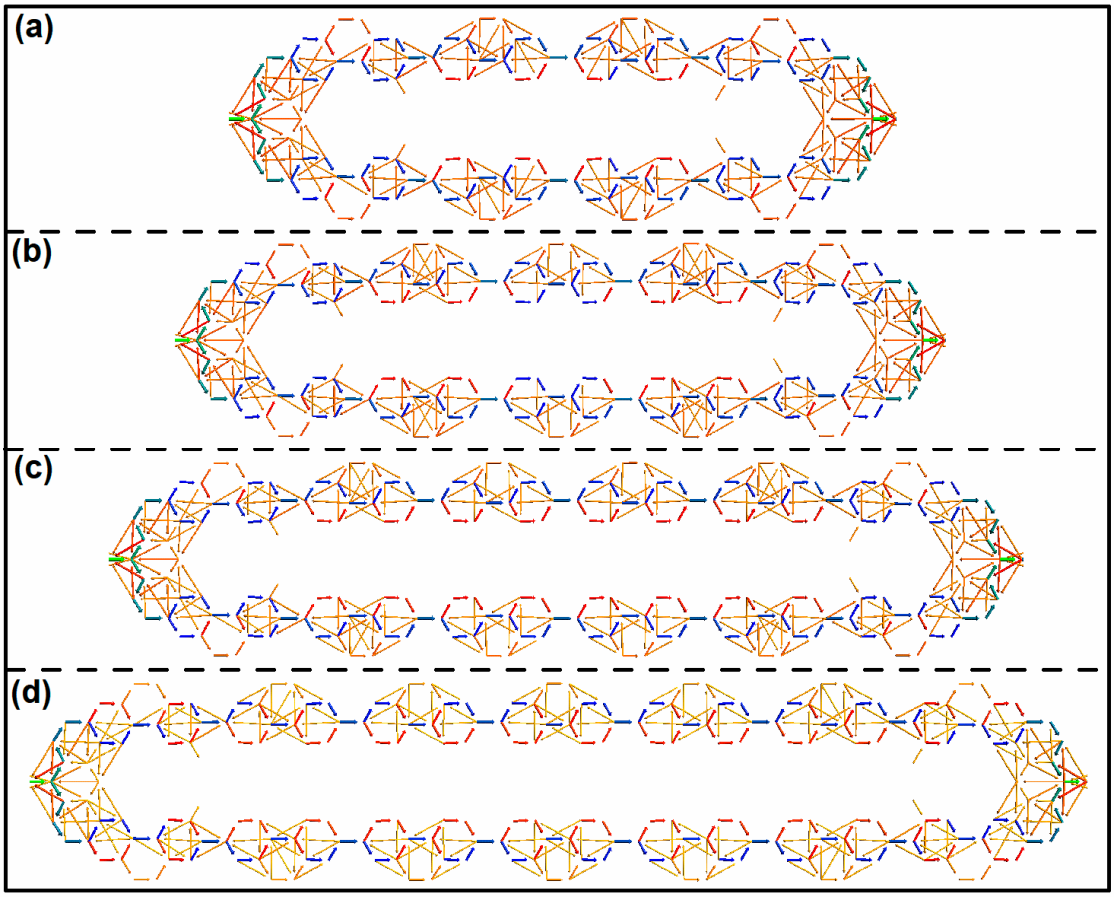

Figure S3 (a-b) Transmission pathways of Device C_2N ring4, 5, 6 and 7, respectively.

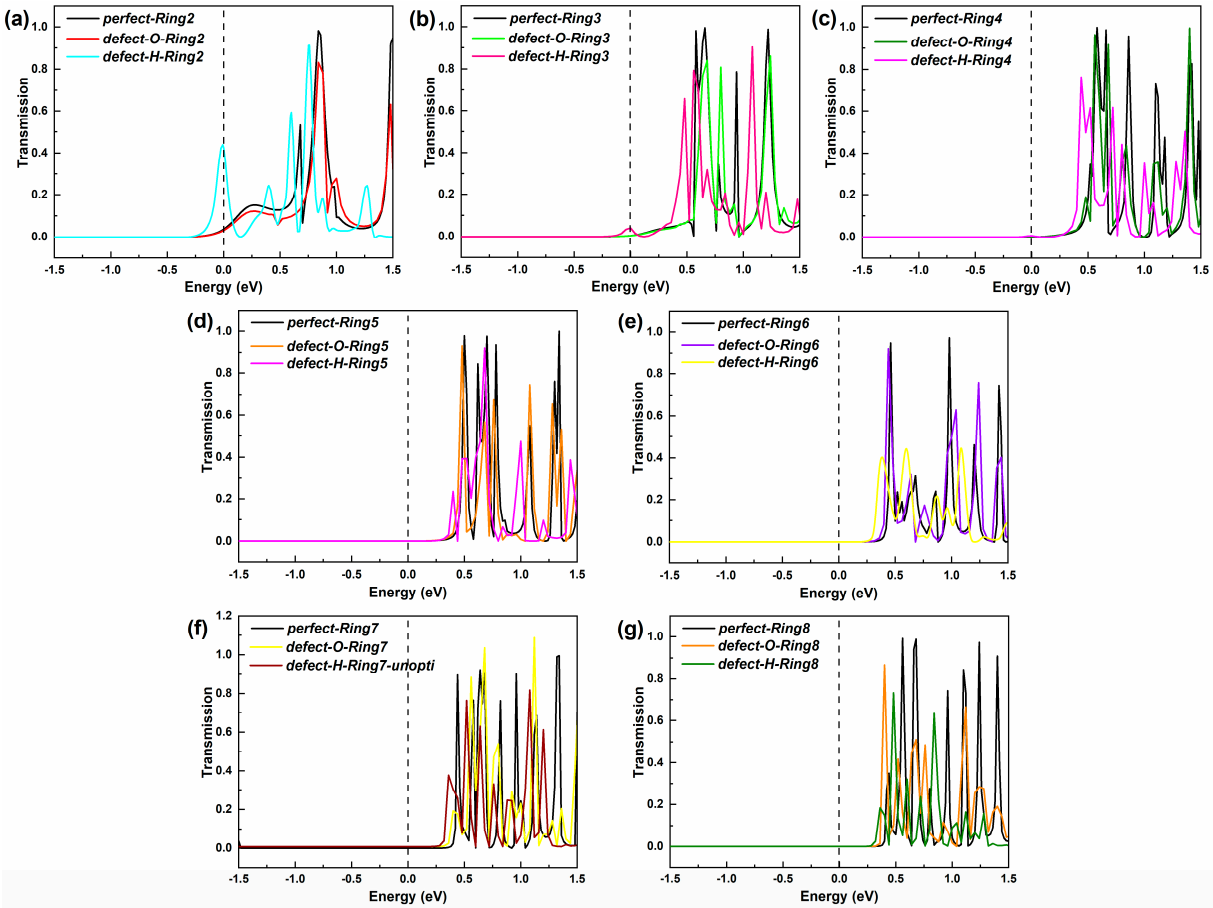

Figure S4 (a-g) Comparison of electron transmission spectrum around E_F of the C_2N rings chains with no defect, O and H impurities for Device C_2N ring 2, 3, 4, 5, 6, 7 and 8, respectively.

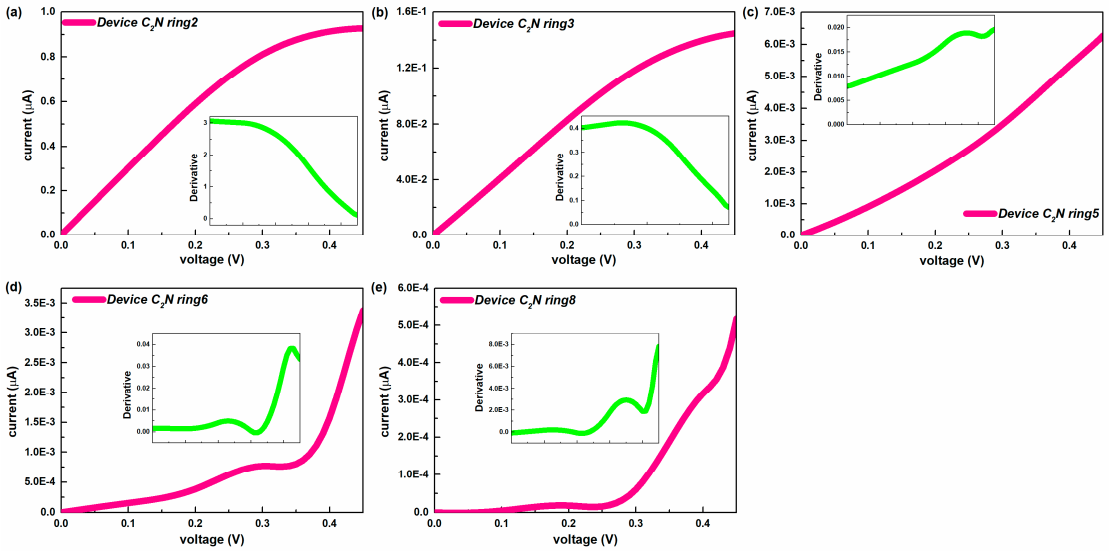

Figure S5 (a-e) I-V curves of Device C_2N ring2, 3, 5, 6, 8, respectively. Each inset shows the first derivative of corresponding I-V curve at biases, representing the growth rate of the current with the bias.

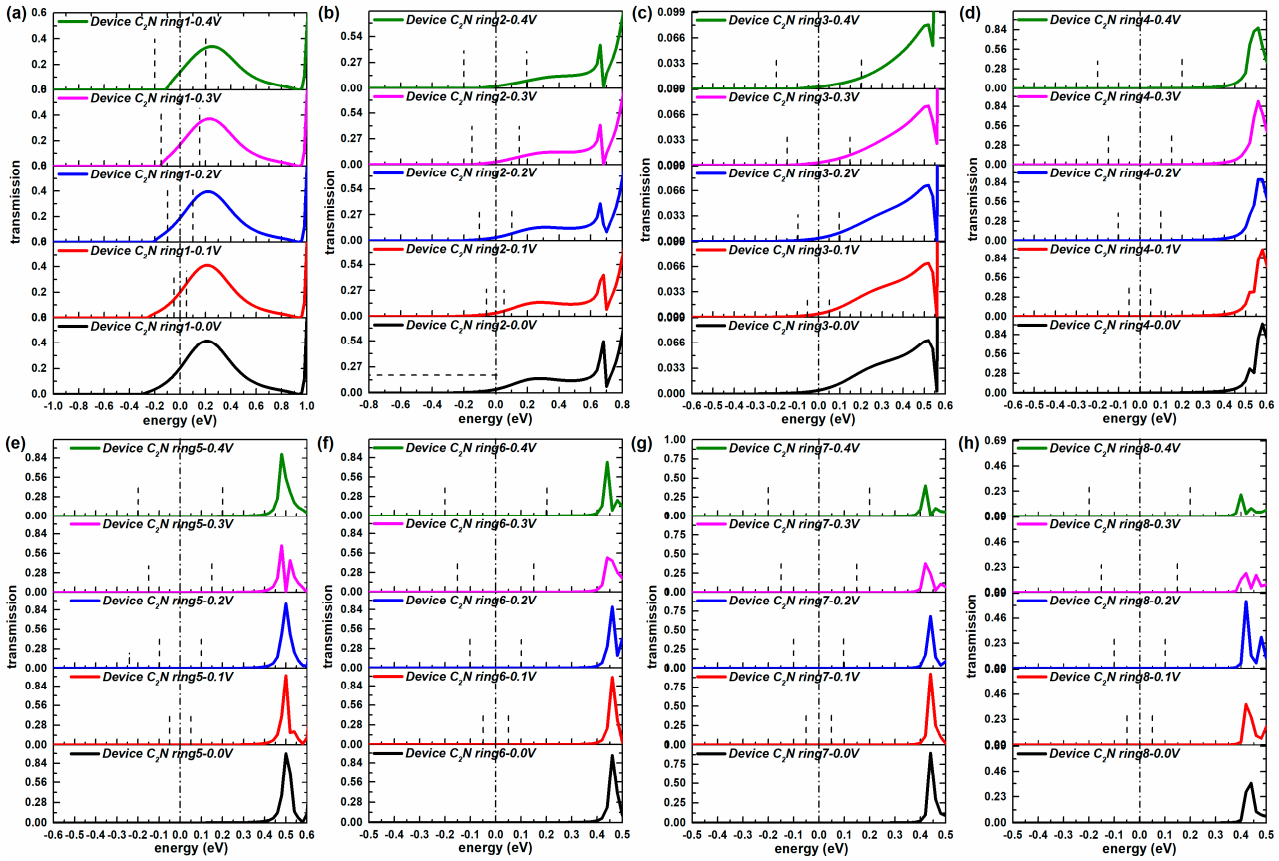

Figure S6 (a-h) Transmission spectrum within wider energy ranges at 0V, 0.1V, 0.2V. 0.3V and 0.4V of Device C_2N ring1-8, respectively.

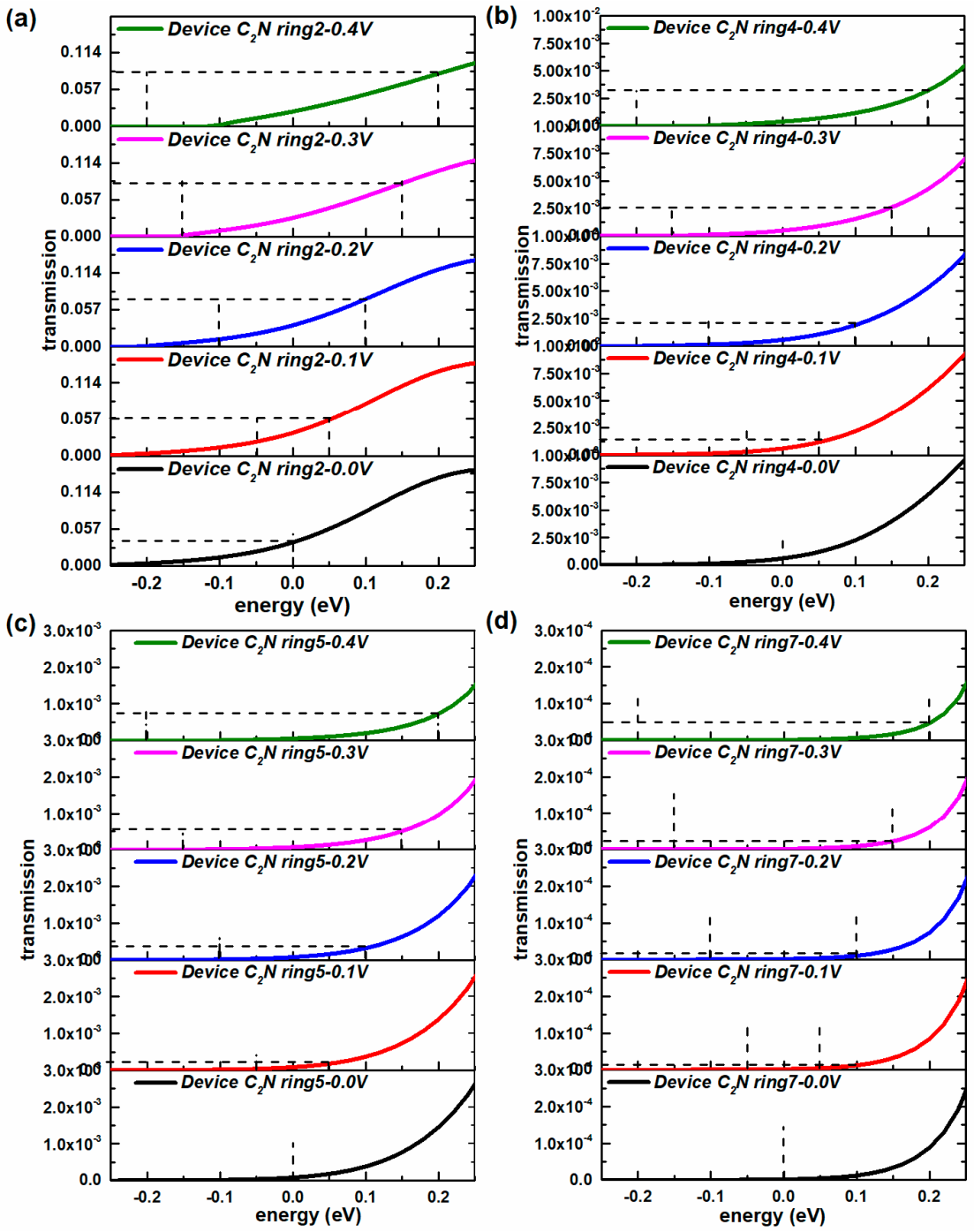

Figure S7 (a-d) Transmission spectrum within narrower energy ranges at 0V, 0.1V, 0.2V. 0.3V and 0.4V of Device C_2N ring2, 4, 5 and 7, respectively.

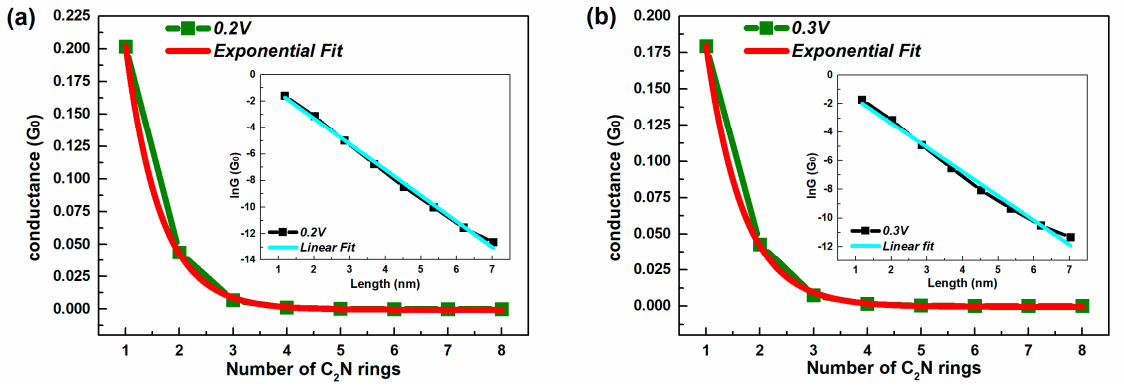

Figure S8 (a-b) Conductance as a function of number of C_2N rings with an exponential fit at 0.2V, and 0.3V, respectively. Each inset exhibits the corresponding lnG as a function of length with a linear fit.