Is the Antiresonance in Meta-Contacted Benzene Due to the Destructive Superposition of Waves Traveling Two Different Routes around the Benzene Ring?

Supporting Information –

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APPLICATIONS OF PATH DECOMPOSITION APPROACH WITH DIFFERENT SCISSOR-CUTTING SCENARIOS

Here we present the results of the path decomposition approach in Fig. 4 in the main text with different scissor-cutting scenarios and with different couplings between molecule and contacts. The left column of Fig. S1 summarizes the comparison of the transmission spectra obtained from the decomposition approach (purple plots) with the original full molecule. In Fig. S1, the coupling strength between the benzene molecule and contacts is set to $\gamma = 0.01\beta$. Path-dependent partial transmissions are shown in the middle column of Fig. S1. We can see that the decomposition approach gives resonances at the mid-gap ($E = \varepsilon_\alpha$) instead of the antiresonances calculated with the original full molecule. In addition, the phase difference between two pathways θ shown in the right column of Fig. S1 does not give π at the mid-gap ($E = \varepsilon_\alpha$).

Figure S2 presents the same plots as Fig. S1 with stronger coupling strengths of the molecule with contacts set to $\gamma = 0.50\beta$. We can see that the transmission spectra based on the decomposition approach with large transfer integral (e.g. $\beta_{23} = 0.9\beta$) gives the similar behavior to the exact solution around the antiresonance at $E = \varepsilon_\alpha$, while it still presents non-negligible mismatch from the exact solution.

APPLICATION OF SCISSORS-CUTTING SCENARIO TO [18]ANNULENE

In addition to the benzene in Fig. 2 in main text, we apply the scissor-cutting approach to [18]Annulene. For simplicity, we consider only π-orbitals within the nearest neighbor approximation as in the main text. The transfer integral is set to β. The homogeneous on-site energy is set to ε_α. Two contacts within the wide-band-limit (WBL) having $\Sigma_{\mathrm{L/R}} = -i0.01\beta$ are attached to site 1 and 9. The transfer integral between site 3 and 4 (β_{34}) is attenuated. The transmission spectra of [18]Annulene with different transfer integral values β_{34} are summarized in Fig. S3. The antiresonance at the mid-gap remains intact during the attenuation, even after the complete attenuation of the bond.

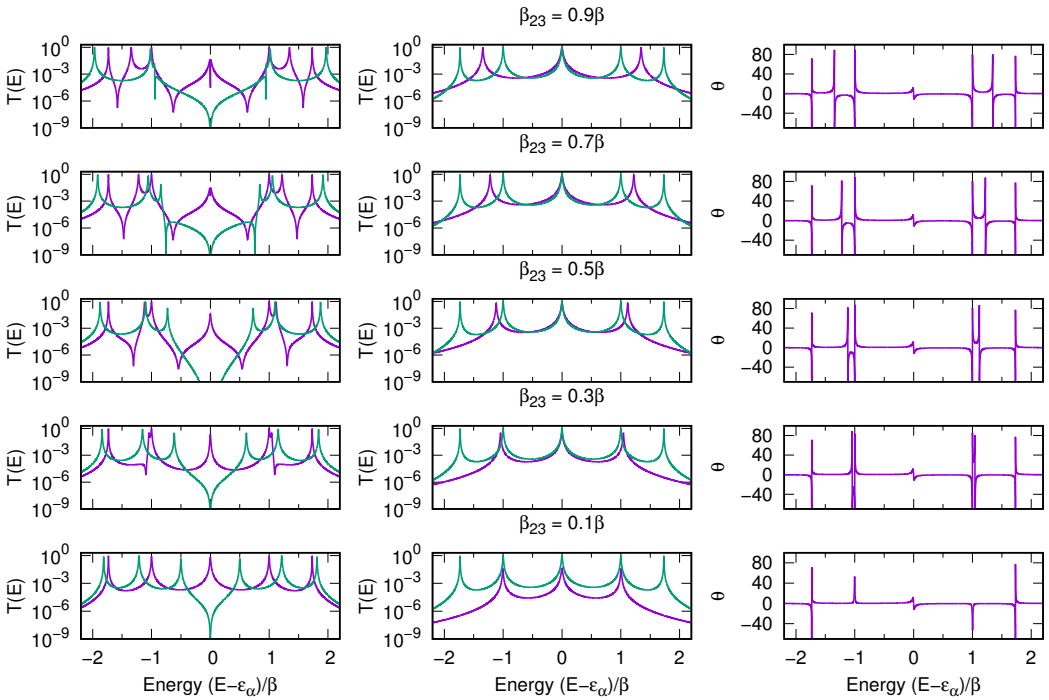

Figure S1: A path decomposition approach with different scissor-cuttings; $\beta_{34} = 0.1\beta, 0.3\beta, 0.5\beta, 0.7\beta$, and 0.9β with weak contact-molecule coupling ($\gamma = 0.01\beta$). (Left column) Comparison of the transmission spectra obtained from the decomposition approach (purple plots) with original full molecule (green plots). (Middle column) Transmission spectra for fragments corresponding to path A (purple plots) and B (green plots). (Right column) Relative phase shift between the upper pathway (Path A) and the lower pathway (Path B).

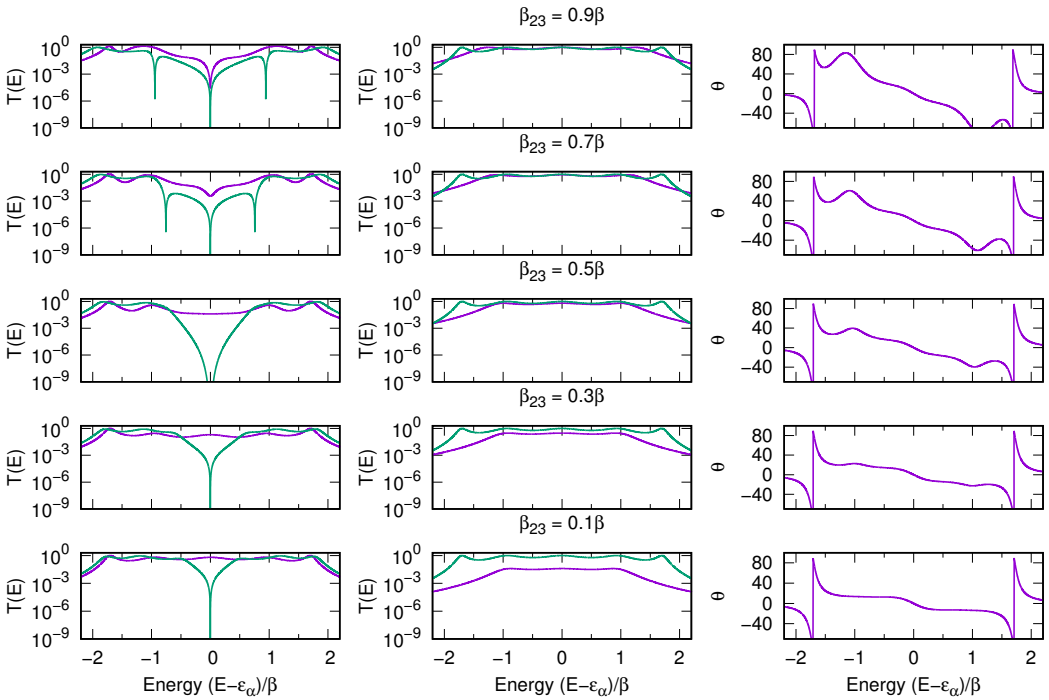

Figure S2: A path decomposition approach with different scissor-cuttings; $\beta_{34} = 0.1\beta, 0.3\beta, 0.5\beta, 0.7\beta$, and 0.9β with strong contact-molecule coupling ($\gamma = 0.50\beta$). (Left column) Comparison of the transmission spectra obtained from the decomposition approach (purple plots) with original full molecule (green plots). (Middle column) Transmission spectra for fragments corresponding to path A (purple plots) and B (green plots). (Right column) Relative phase shift between the upper pathway (Path A) and the lower pathway (Path B).

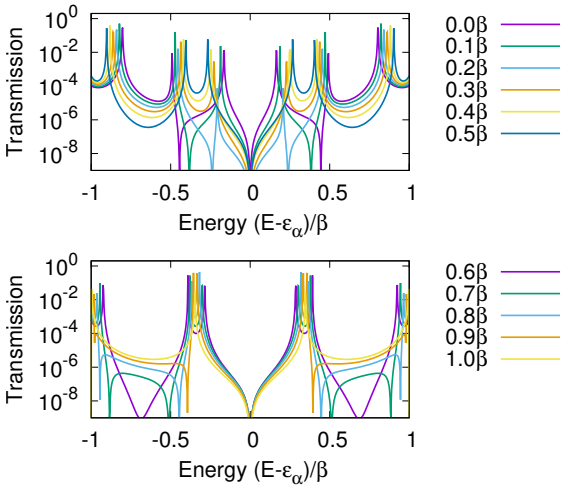

Figure S3: Transmission spectra for [18]Annulene connected between WBL-based contacts with different transfer integral β_{34}. Similar to the case with benzene in main text, the antiresonance remains during the attenuation of the bond.