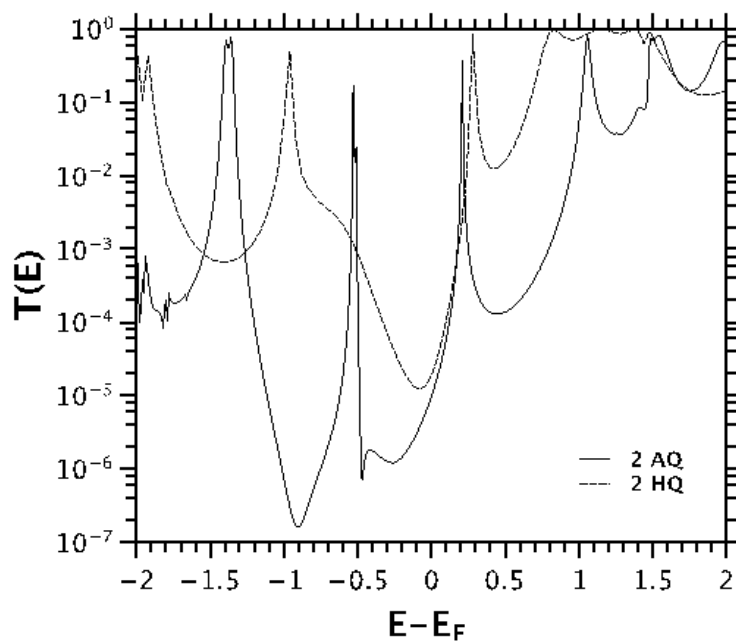
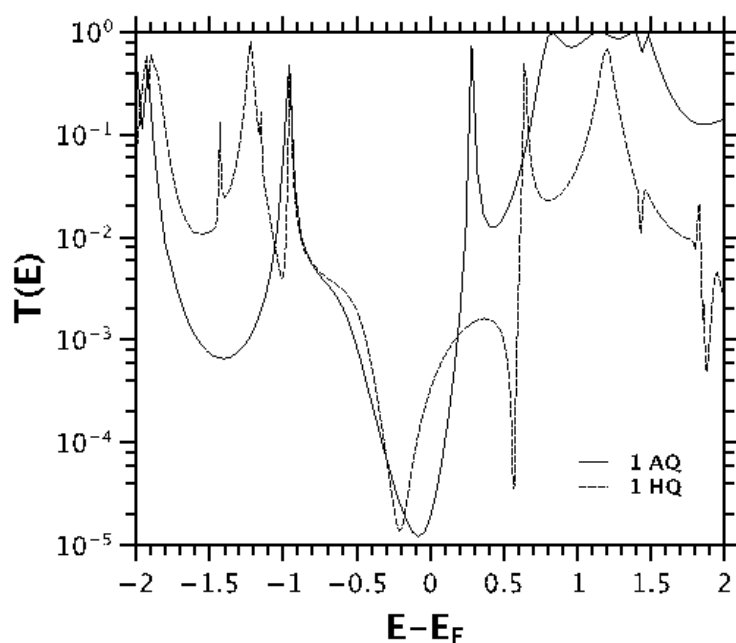


## Supplementary Material



**Fig S1:** Comparison of the DFT non-equilibrium Greens function (NEGF) formalism calculated energy dependent transmission coefficients for **2** of the anthraquinone (AQ) and hydroquinone (HQ) modification of **2**.



**Fig S2:** Comparison of the DFT non-equilibrium Greens function (NEGF) formalism calculated energy dependent transmission coefficients for **1** of the anthraquinone (AQ) and hydroquinone (HQ) modification of **1**.