Supplementary Information:

Examining Energy Storage Potential in Weakly Polar Nematic Liquid Crystals Infused with Anthraquinone Dye: A Comprehensive Approach

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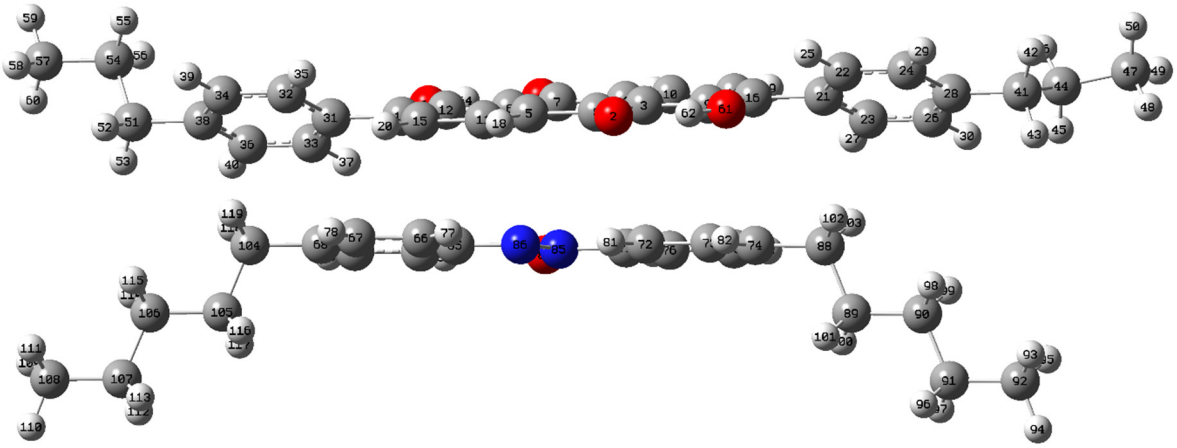

Figure S1: Initial structure of the dye-NLC complex used in the DFT calculations.

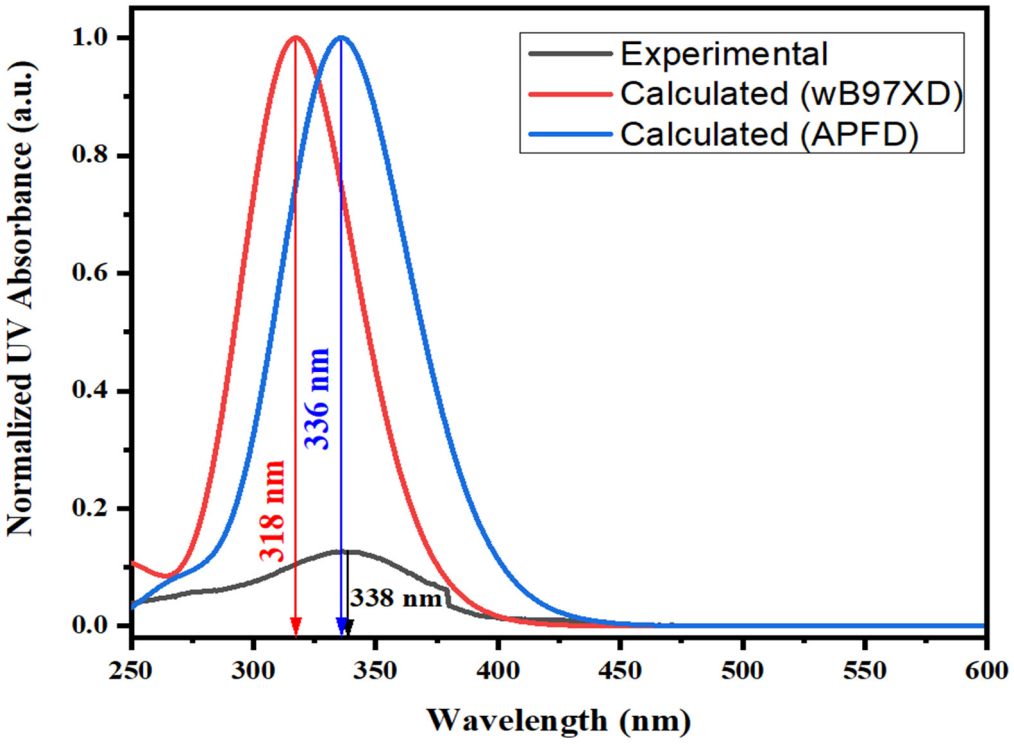

Figure S2: A comparison between the UV-Vis spectra of pure D5AOB liquid crystal obtained experimentally and those calculated at different levels of theory. To facilitate comparison, all three spectra have been normalized. Notably, a 20 nm shift is observed between the experimental and wB97XD/6-311++G(d,p) calculated spectra. However, this shift decreases to 2 nm in the spectra calculated using the APFD/6-311++G(d,p) level of theory, which falls within an acceptable range.

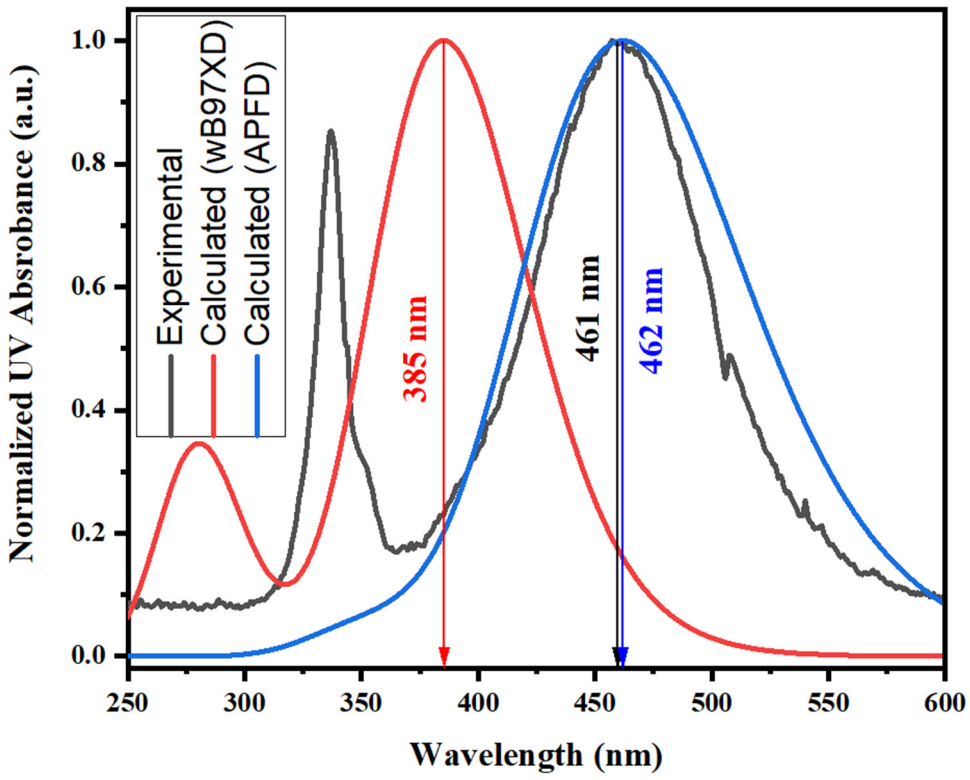

Figure S3: A comparison of UV-Vis spectra for the anthraquinone dye (26B3OH), showcasing both experimental and calculated spectra. All three spectra have been normalized for ease of comparison. Notably, there is an approximately 76 nm shift between the experimental spectra and those calculated at the wB97XD/6-311++G(d,p) level of theory. However, when employing the APFD/6-311++G(d,p) level of theory, this shift decreases to just 1 nm, well within an acceptable range.

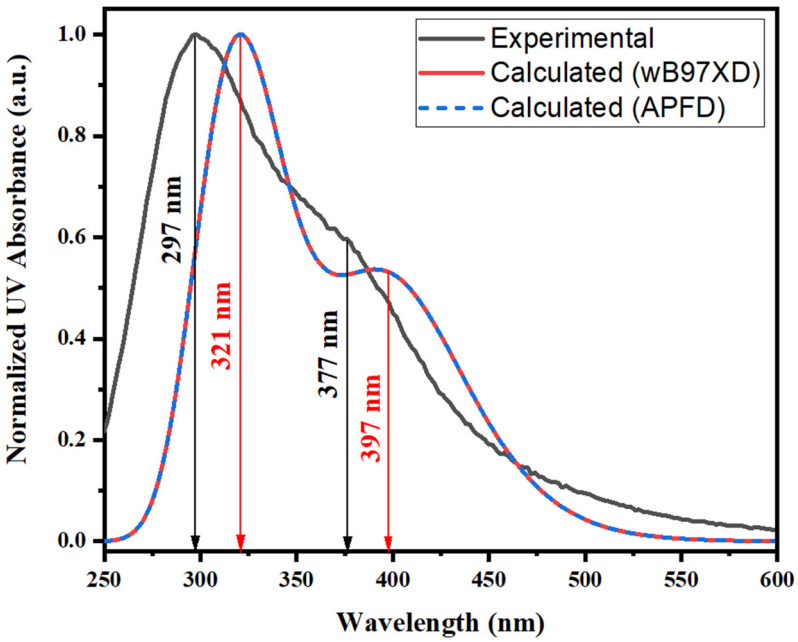

Figure S4: Comparison of experimental and calculated UV-Vis spectra for D5AOB+26B3OH complex. All three spectra are normalized to unity for comparison purposes. A shift of about 24 nm from the main peak and 20 nm from the shoulder peak from experimental spectra can be seen in the spectra calculated at wB97XD/6-311++G(d,p) APFD/6-311++G(d,p) level of theory. In the case of the Dye-LC complex, both calculated spectra are identical thus they are overlapping in the above figure.