

Supporting Information for:

Coupling Between a Molecular Charge-Transfer Exciton and Surface Plasmons in a Nanostructured Metal Grating

Natalia Azarova,¹ Andrew J. Ferguson,² Jao van de Lagemaat,² Elisabeth Rengnath,¹ Wounjhang Park,¹ Justin C. Johnson^{2,*}

¹Department of Electrical, Computer & Energy Engineering, University of Colorado, Boulder, CO 80309

²National Renewable Energy Laboratory, 15013 Denver West Pkwy, Golden, CO 80401

I. Fits to simulated PTCDA/grating absorption data

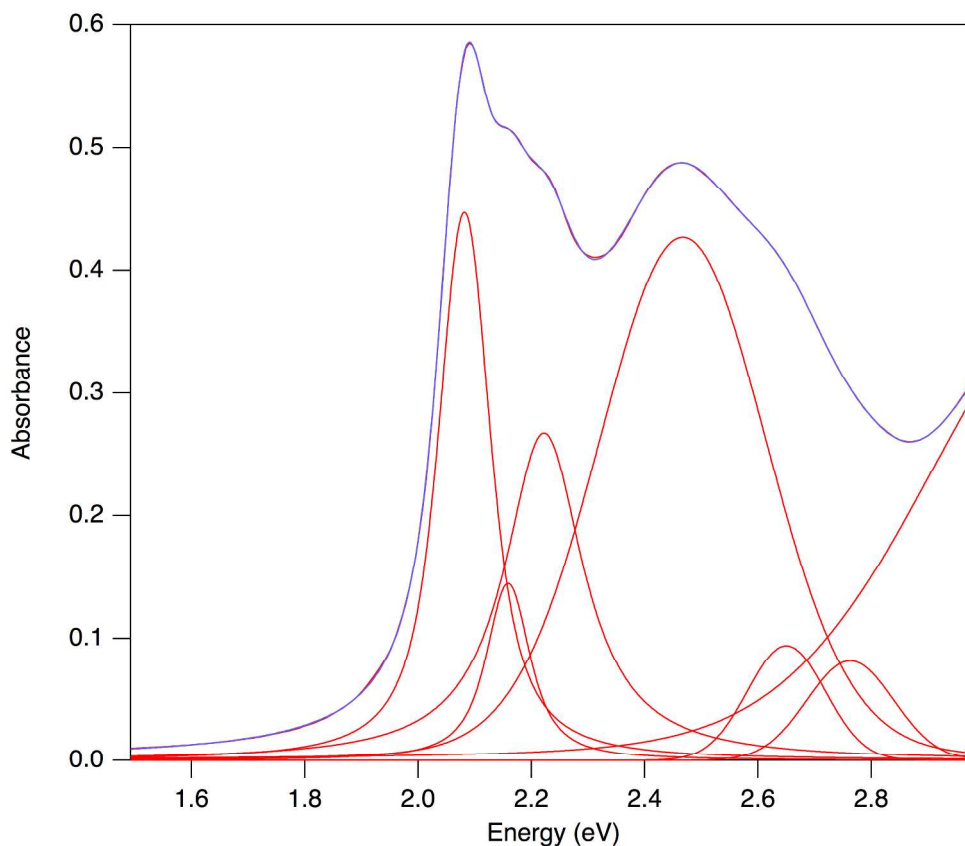


Figure S1. Simulated absorption spectrum as a function of light energy of PTCDA on a silver grid at a 5 degree incident angle. The fit and the simulated spectrum coincide. The positions, width and intensities of the Lorentzian oscillators used to fit the simulated spectrum are shown in red.

II. PTCDA on glass reflectivity spectrum and fit

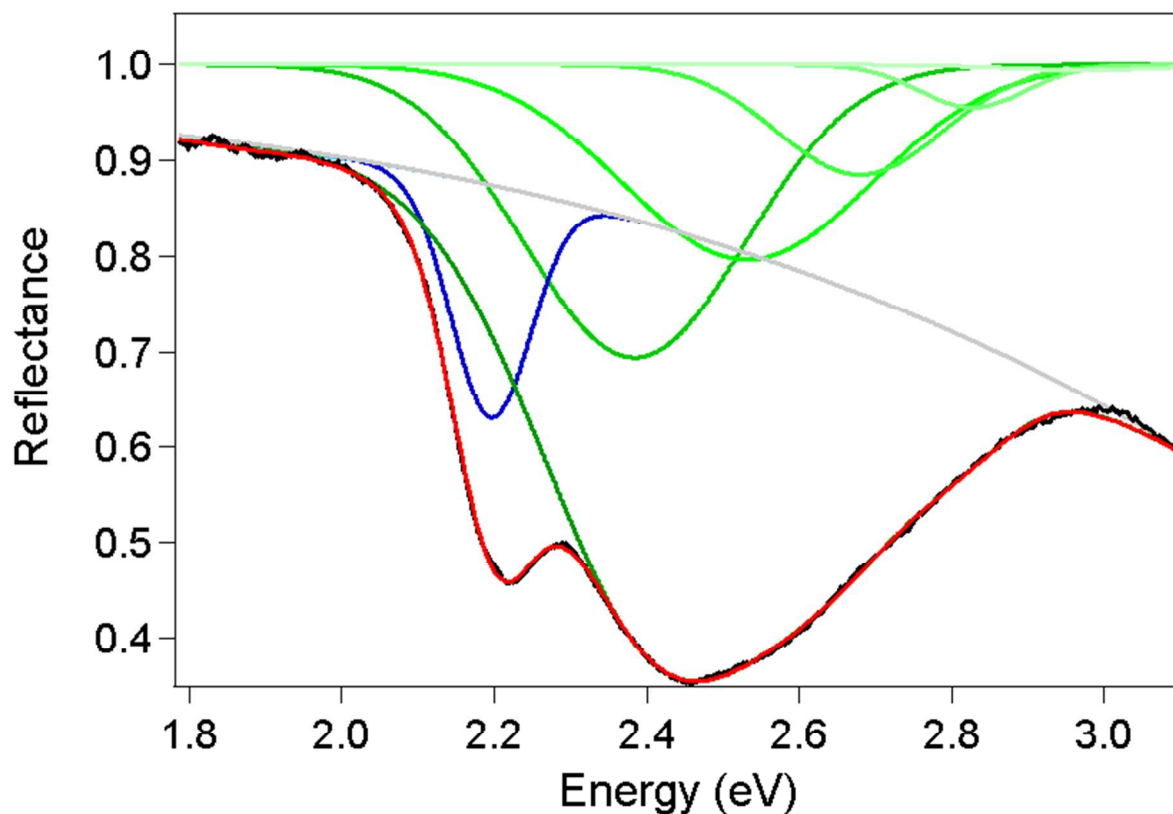


Figure S2. Reflectance data (black) and fits for a 20 nm PTCDA layer on glass. As in the main text, green curves are the vibronic progress of PTCDA (dark green is the sum of the individual components), the blue curve is the CTE band, and the gray curve is a scattering component. A cyan curve, barely visible near 2.0 eV, is the low energy CTE band (sometimes referred to as self-trapped CTE), which varies in intensity on different samples but in general is needed to produce a satisfactory fit.

III. Fluorescence data for PTCDA/50 nm Al₂O₃/grating sample

IV.

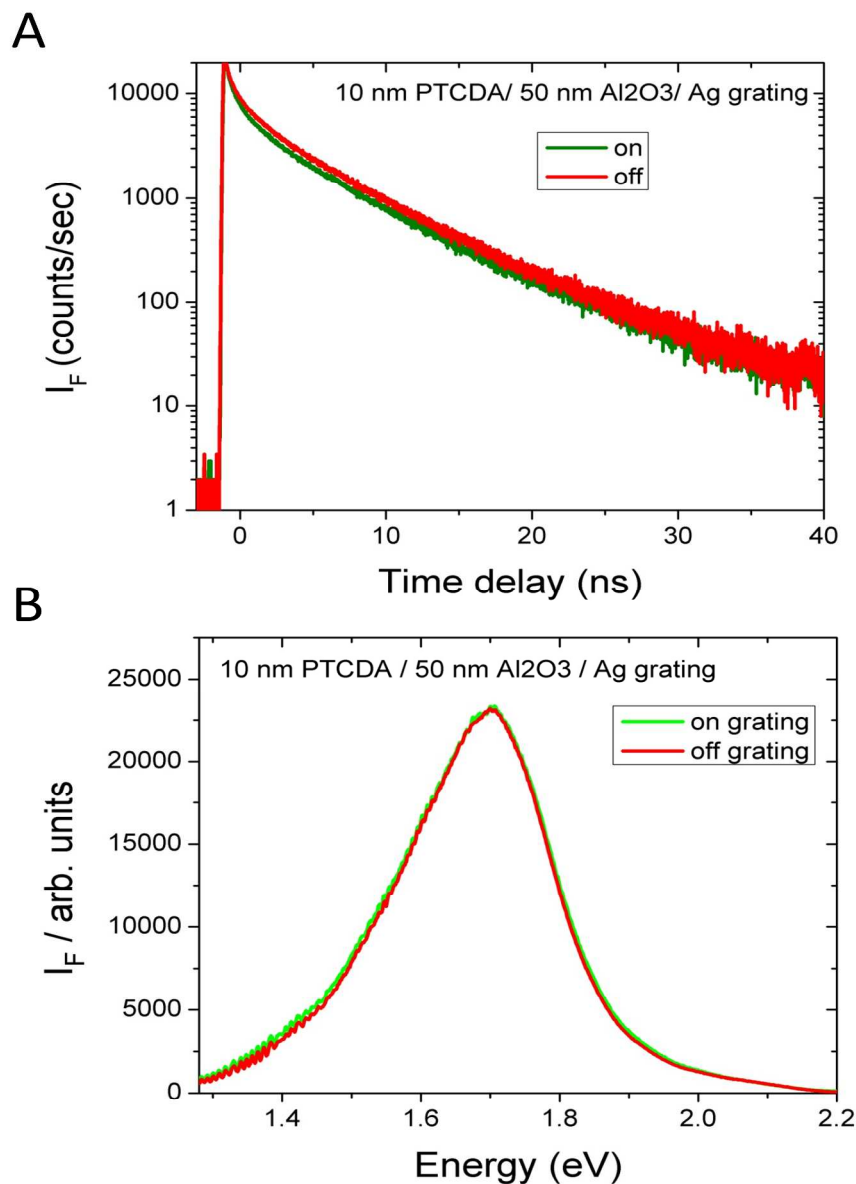


Figure S3. (A) TCSPC data collected at 1.45 eV for PTCDA separated from the grating by a 50 nm ALD Al₂O₃ spacer. These measurements were collected via time-correlated single photon counting (Becker-Hickl) with 1 nJ pulses at 560 nm and 10 MHz repetition rate (Fianium, SC-450-PP). (B) Steady-state PL for the same sample.

IV. Full fits to PTCDA/grating reflectance data

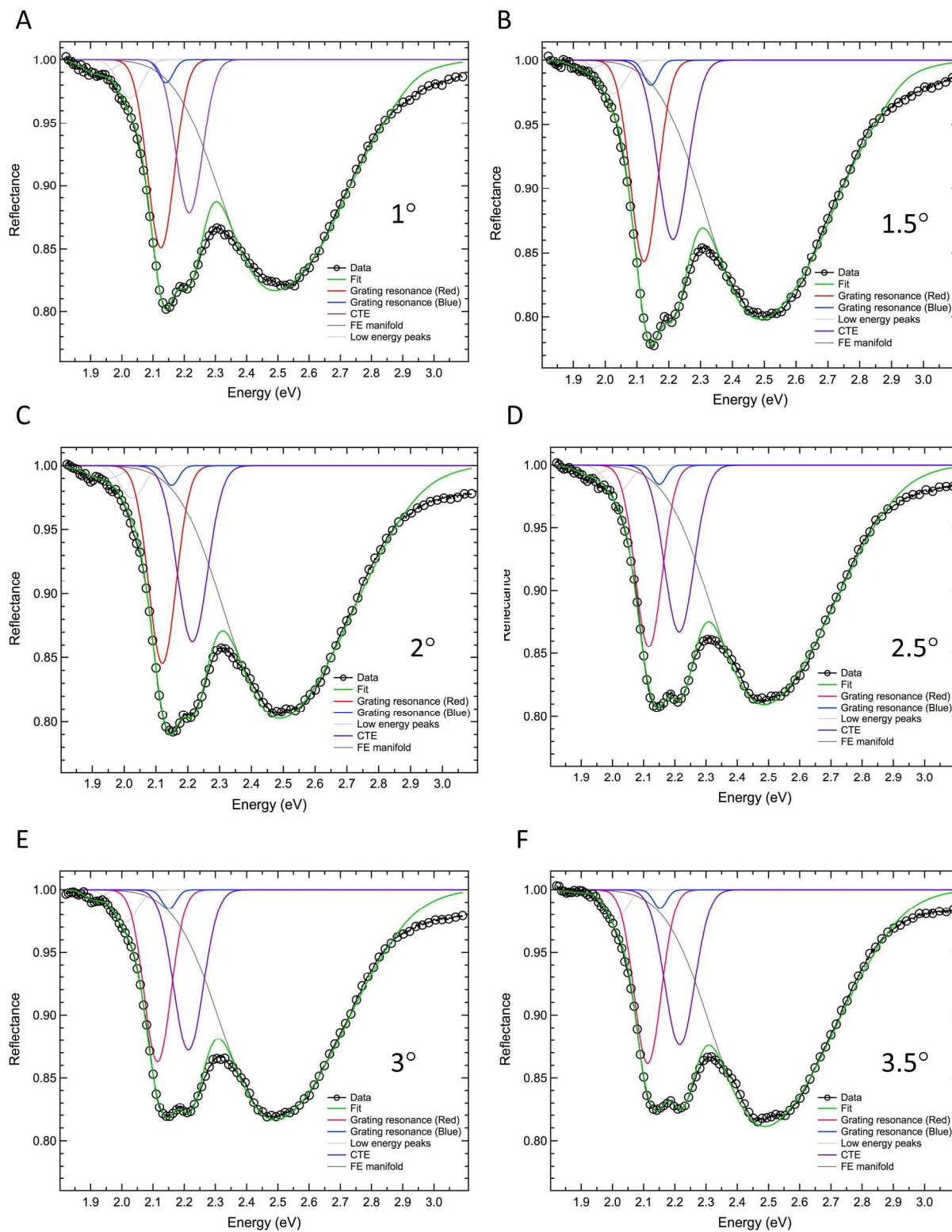


Figure S4. Reflectivity and peaks used in fit of Ag grating/2-5 nm Al_2O_3 /PTCDA samples for incident angles 1 through 3.5 degrees.

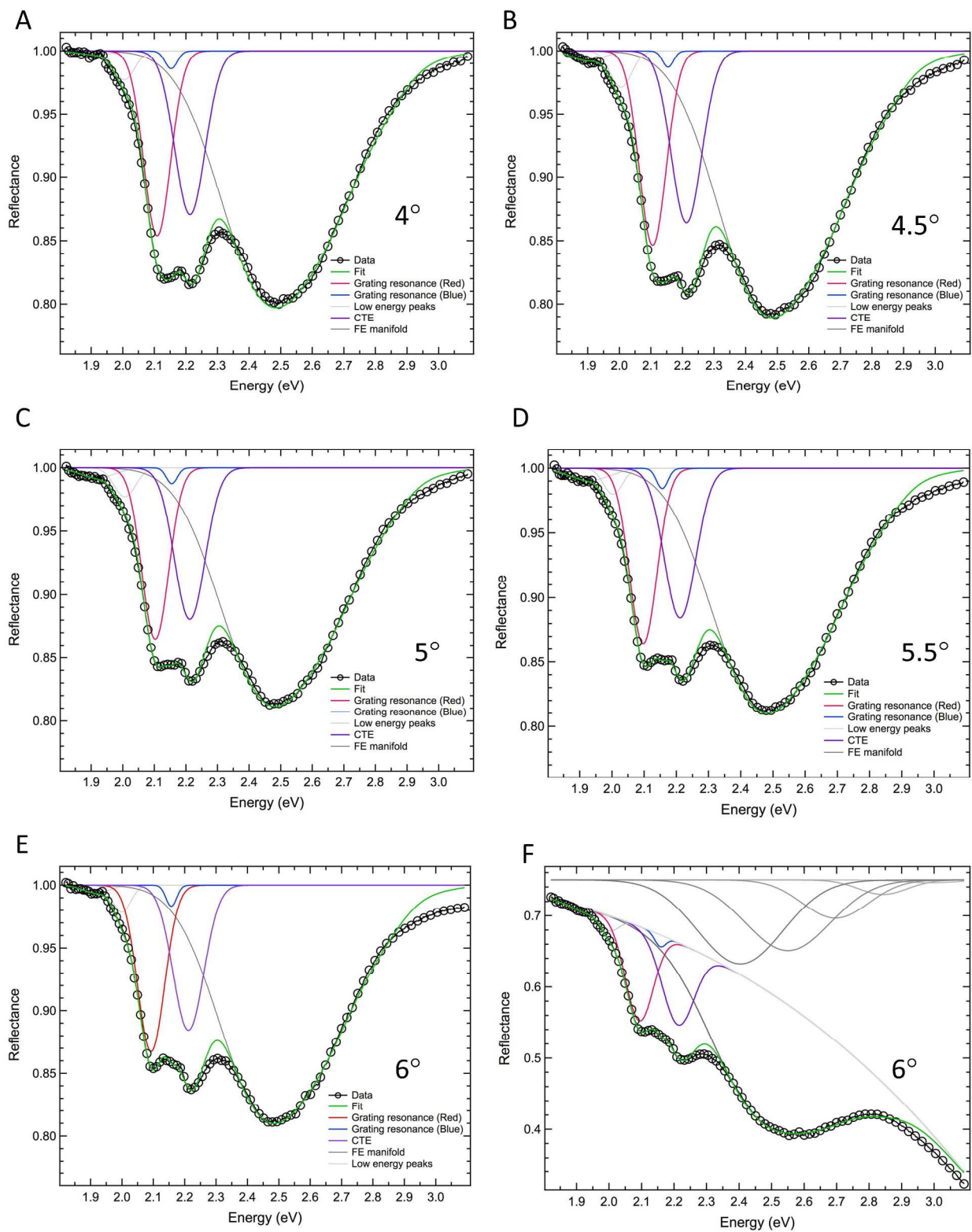


Figure S5. Reflectivity and peaks used in fit of Ag grating/2-5 nm Al_2O_3 /PTCDA samples for incident angles 4 through 6 degrees. The raw data with scattering component for one angle are shown in panel F.

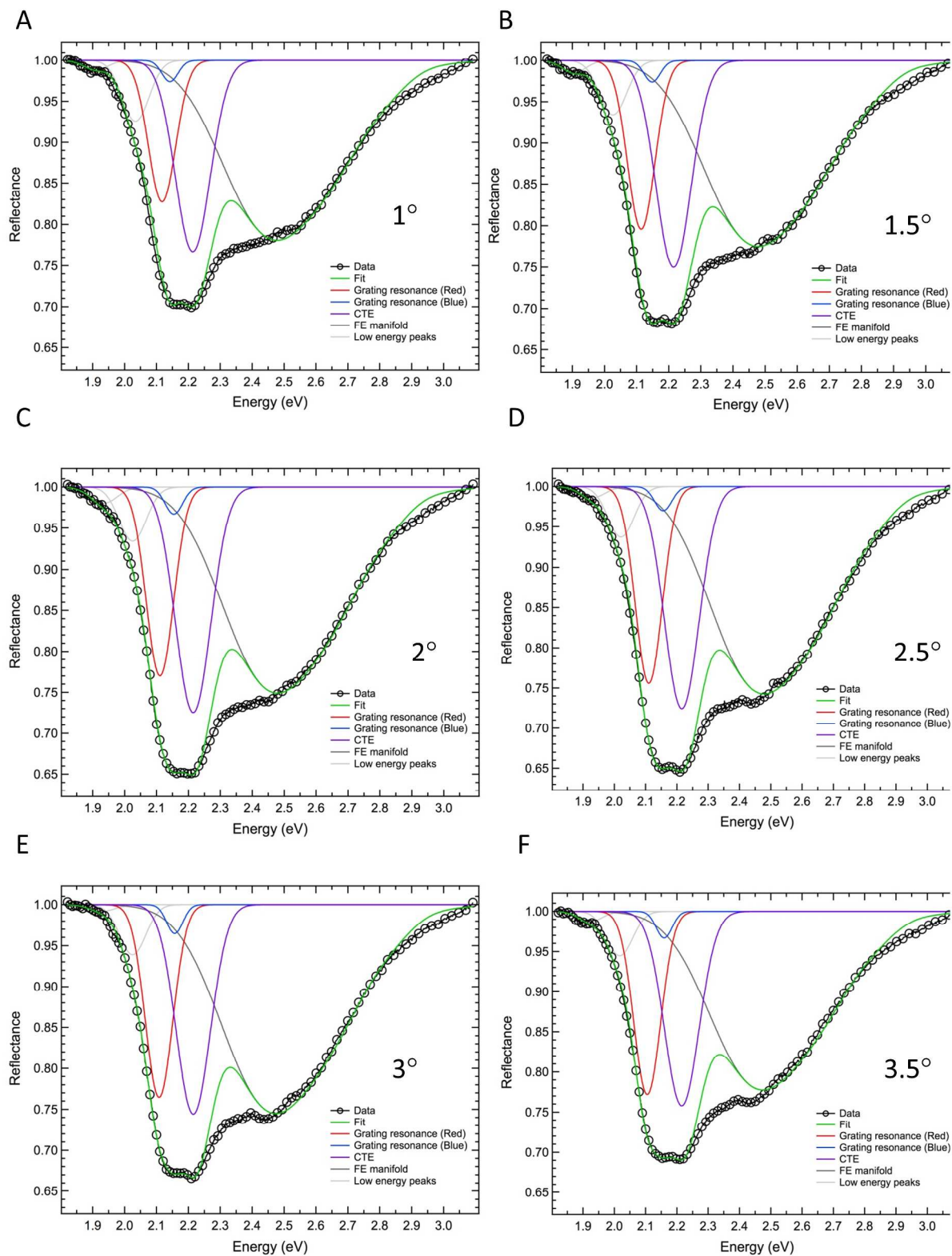


Figure S6. Reflectivity and peaks used in fit of Ag grating/PTCDA samples for incident angles 1 through 3.5 degrees.

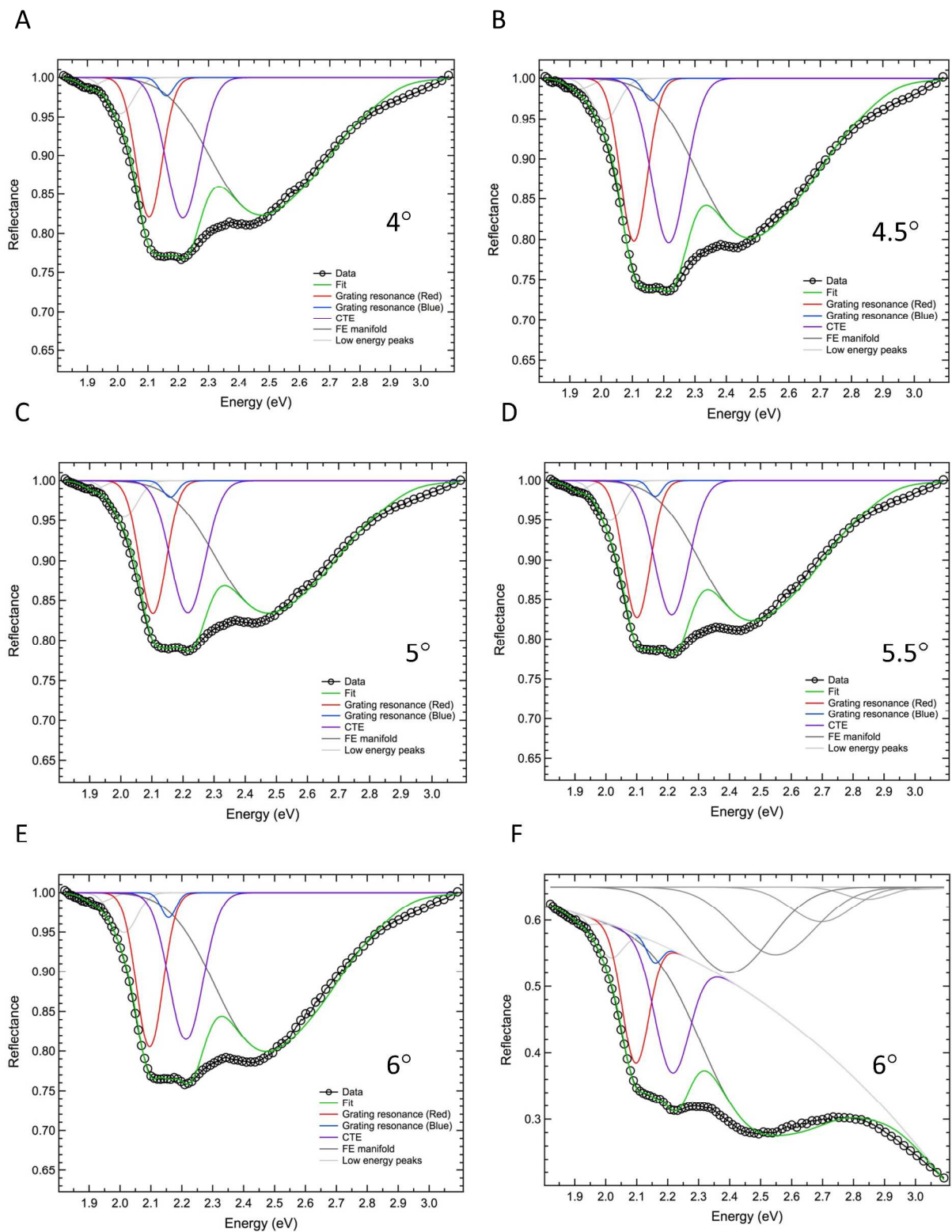


Figure S7. Reflectivity and peaks used in fit of Ag grating/2-5 nm Al₂O₃/PTCDA samples for incident angles 4 through 6 degrees. The raw data with scattering component for one angle are shown in panel F.

V. Peak shifting for PTCDA/grating sample with no Al_2O_3 layer

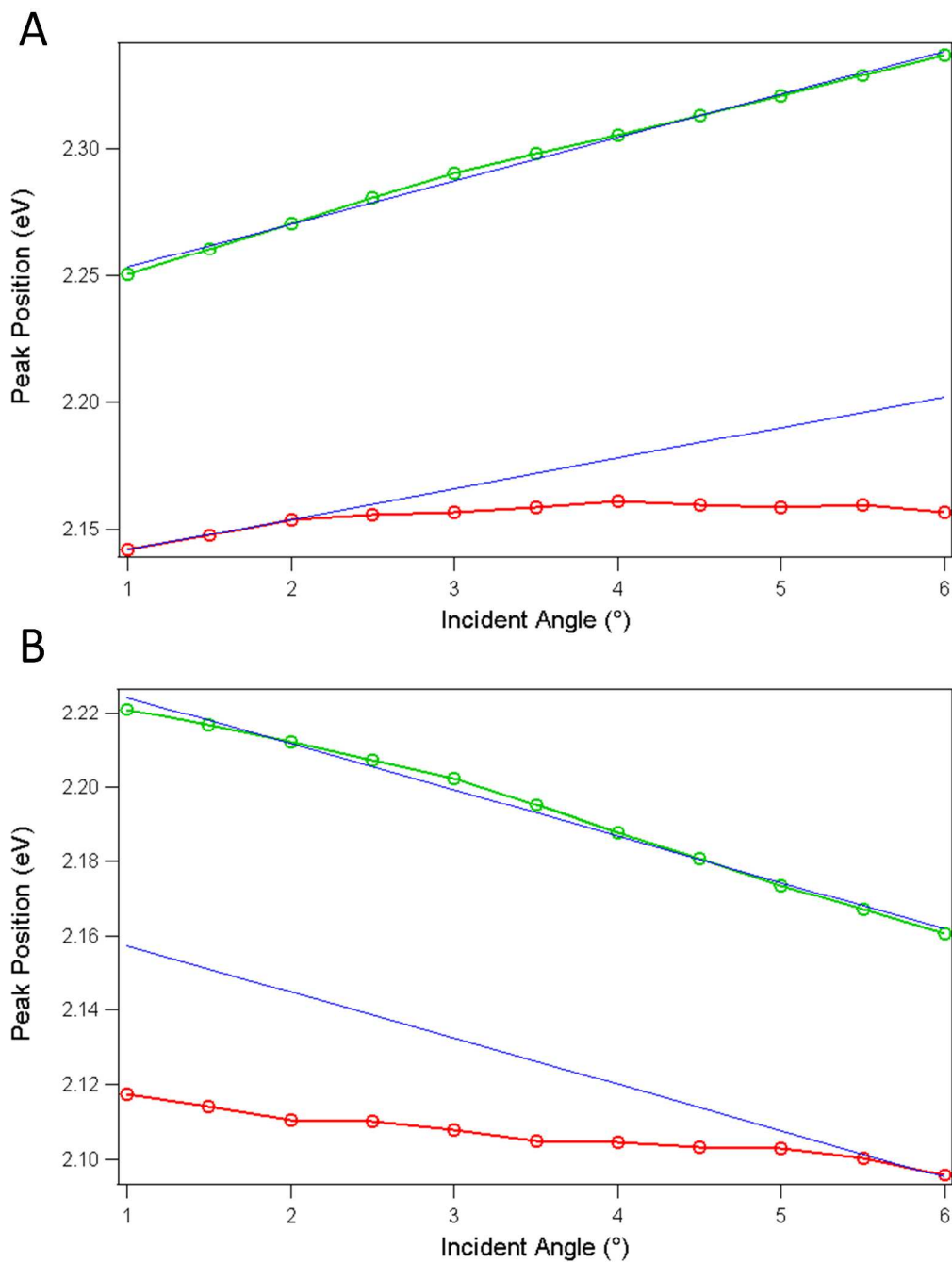


Figure S8. Peak position vs. incident angle for the PTCDA/grating sample similar to that shown in Figures 4A and B of the main text.