Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Inferring Relative Dose-dependent Color Center Populations in Proton Irradiated Thoria Single Crystals using Optical Spectroscopy

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Supplemental Information

Figure S1 shows the electron band structure of pristine thoria calculated using density functional theory with independent particle approximation and the local density approximation (LDA) within Quantum Espresso.

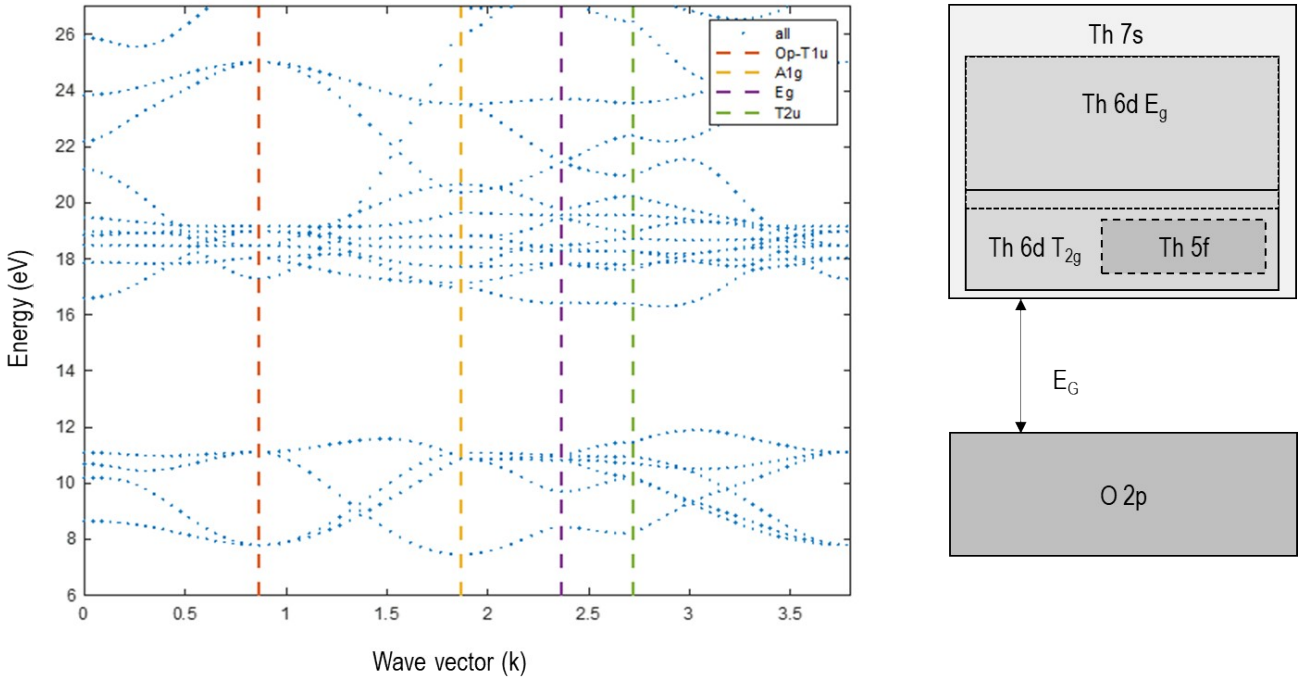

Figure S1. Electron band structure obtained from DFT.

Figure S2 shows a comparison of the calculated electronic band structure between a pristine thoria supercell (Th_8O_{16}) and the newly-created ground and excited states from the F-centers.

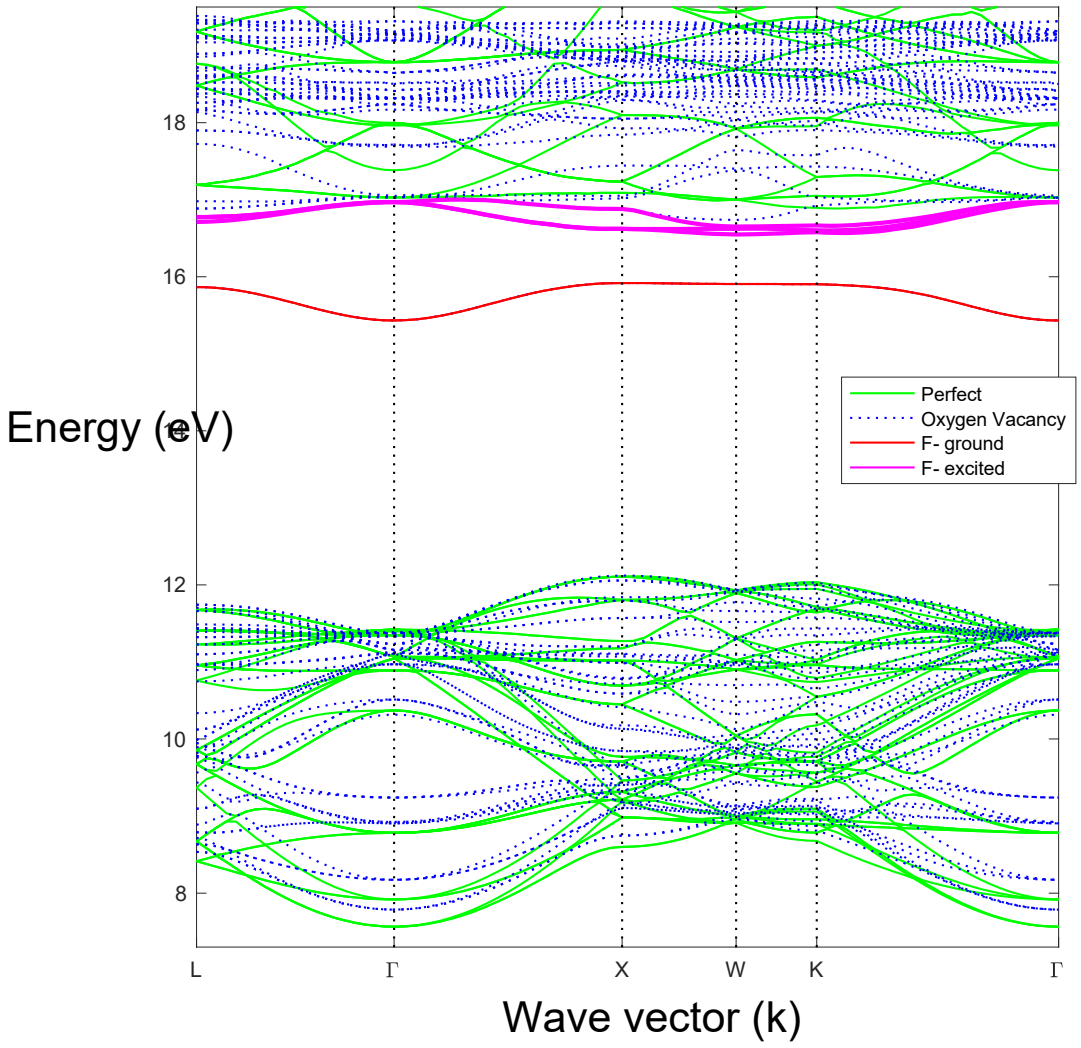

Figure S2. Electronic band structure of a perfect thoria supercell (green lines) along with a supercell containing F-centers. The newly created ground and excited states in the supercell containing the F-centers are shown with the red and magenta curves, respectively.