

Supporting Information

Identification of Interstitial Oxygen Color Centers in CaGdAlO₄

Single Crystals and their Elimination Strategy

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Table S1. System energy and O_i doping energy

Interstice	Average energy of system (eV/atom)	E _f (eV)
Non	-7.503	/
Al-O	-7.366	8.145
Gd/Ca-O	-7.448	-1.201

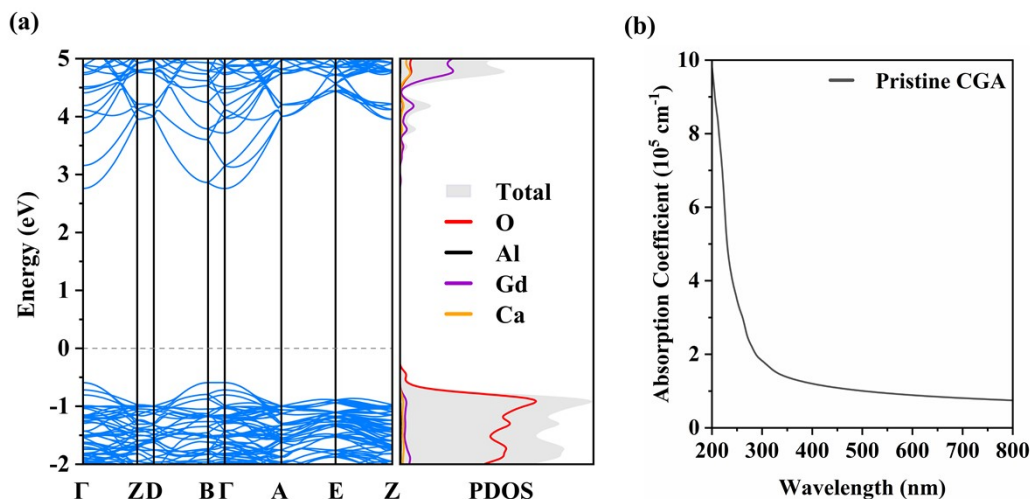


Figure S1. (a) The electronic structure and (b) The absorption spectrum of pristine CGA

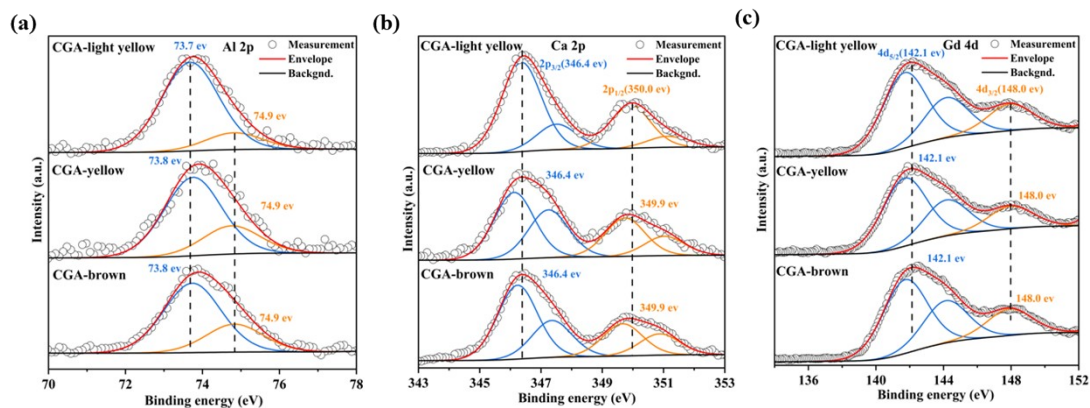


Figure S2. The XPS spectra of (a) Al 2p, (b) Ca 2p, and (c) Gd 4d for the CGA-light yellow, CGA-yellow, and CGA-brown samples.

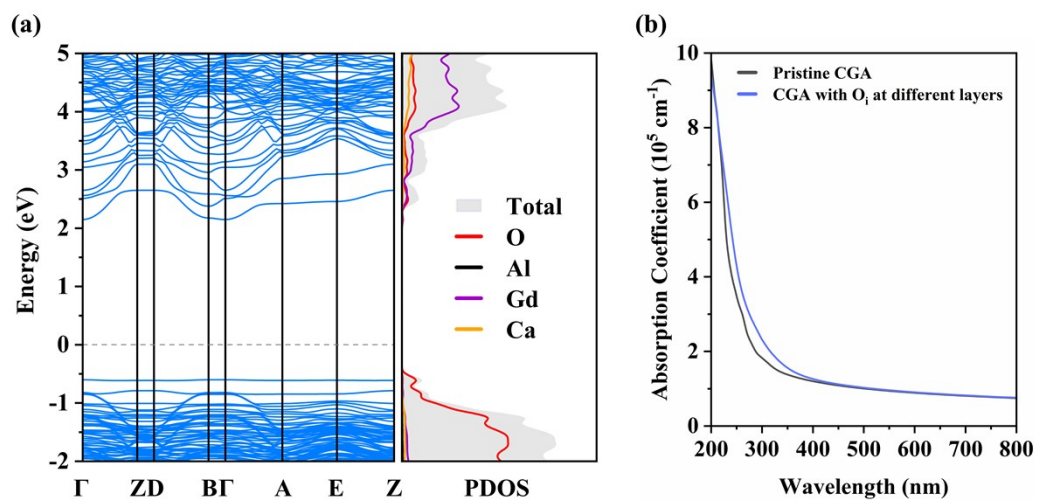


Figure S3. (a) The electronic structure and (b) The absorption spectrum of CGA with O_i at different layers