

Supporting Information
for
Iron-doped β -Ga₂O₃ single crystal: iron occupying site and
optical properties

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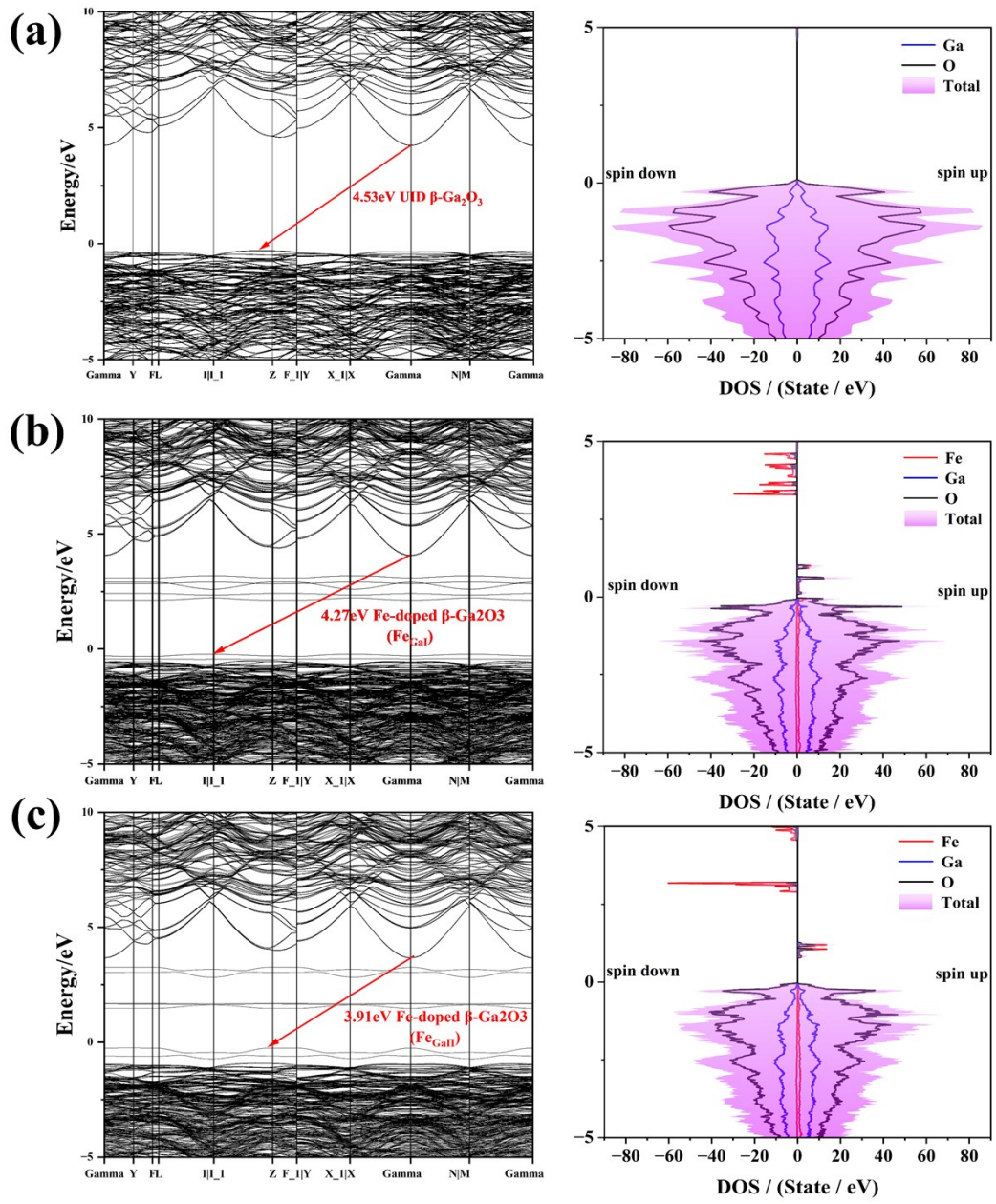


Fig. S1 The bandgap and DOS of the UID $\beta\text{-Ga}_2\text{O}_3$ and Fe-doped $\beta\text{-Ga}_2\text{O}_3$ where (a) UID $\beta\text{-Ga}_2\text{O}_3$ (b) Fe replacing Ga_{I} site and (c) Fe replacing Ga_{II} site.

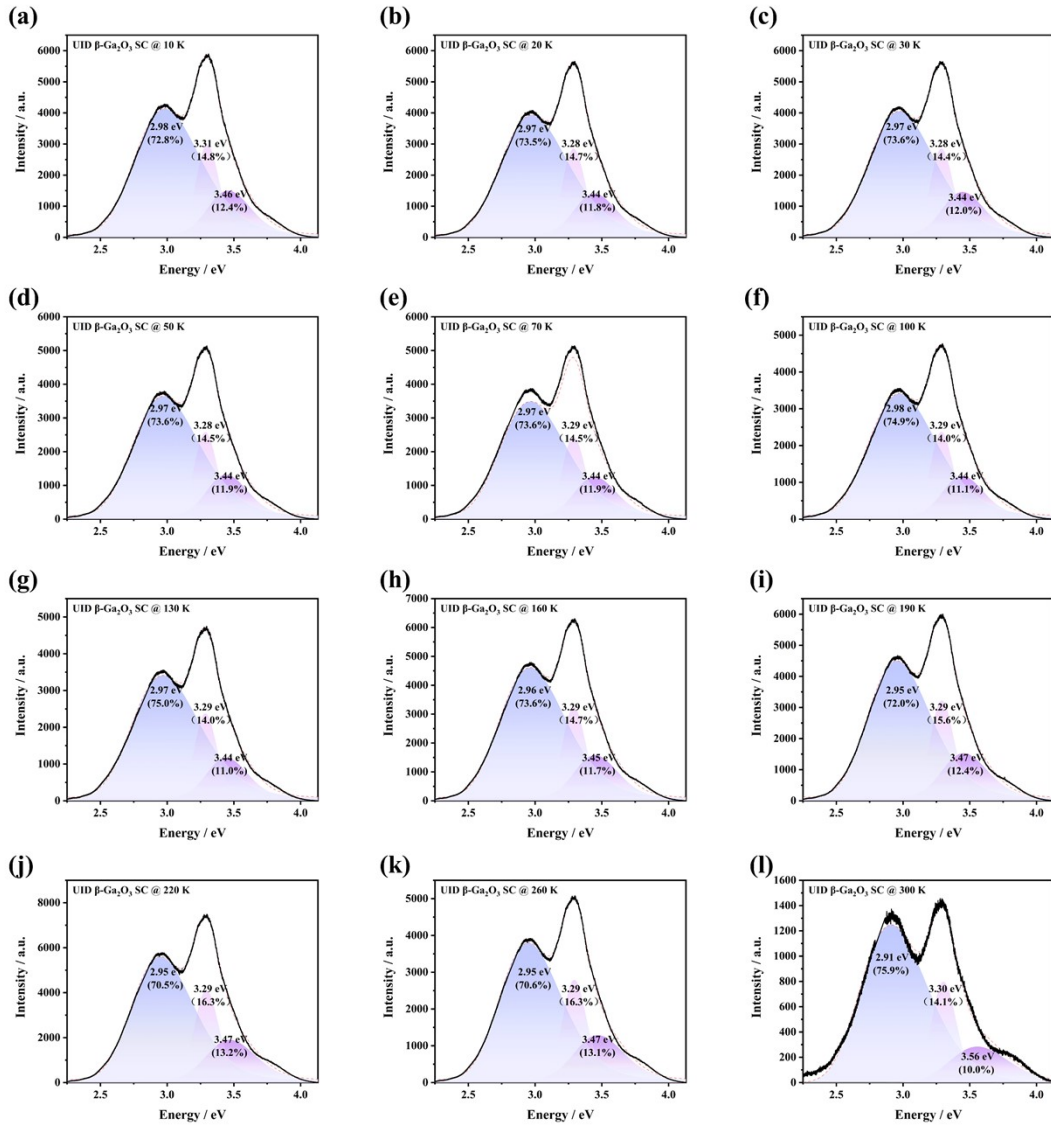


Fig. S2 (a-l) The Gaussian fitting curves of temperature-dependent PL spectra of the UID β -Ga₂O₃ SC from 10 K to 300 K.

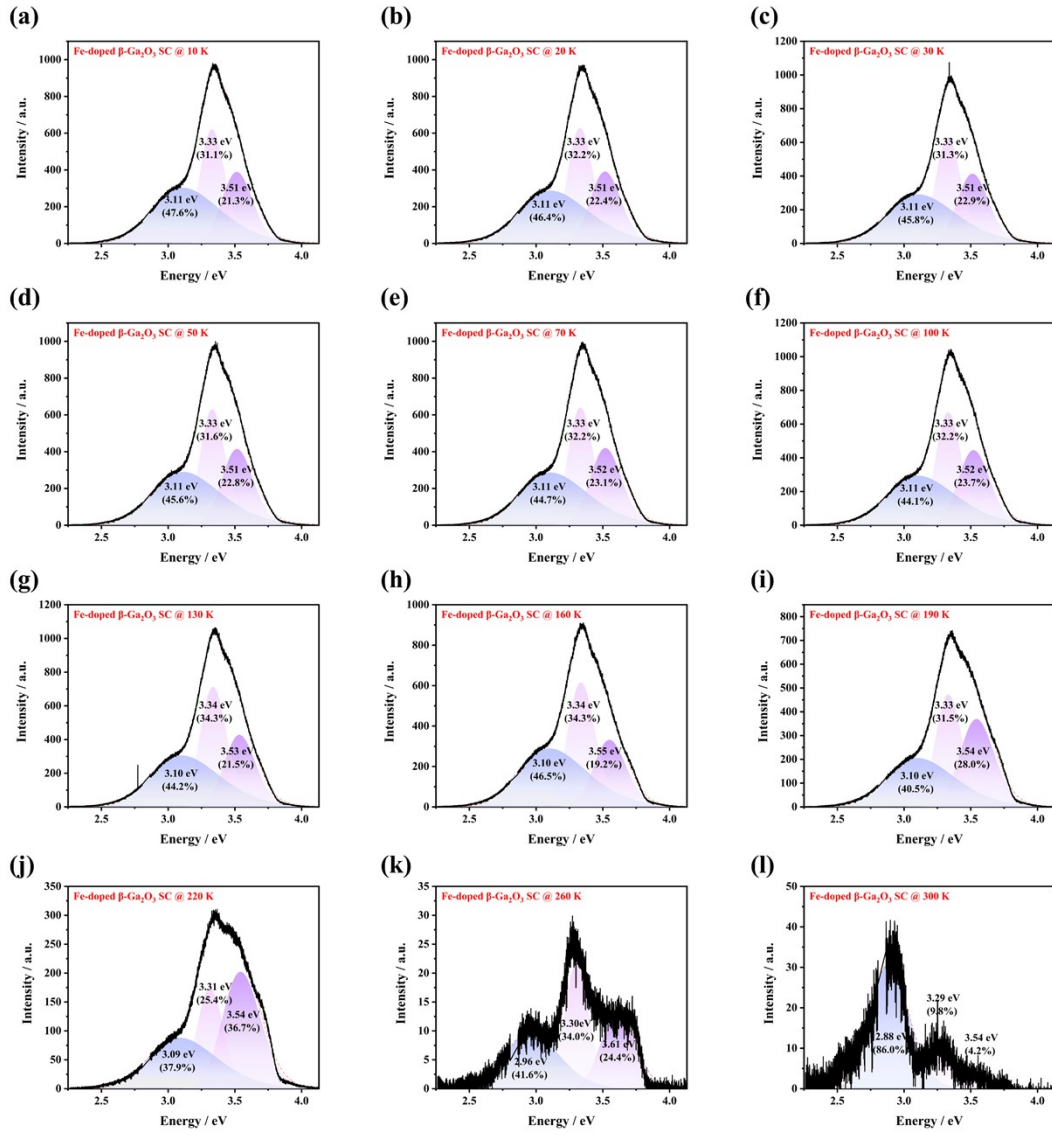


Fig. S3 (a-l) The Gaussian fitting curves of temperature-dependent PL spectra of Fe-doped β -Ga₂O₃ SC from 10 K to 300 K.