

# First-Principle Study of Optical Properties in Erbium-Doped Fibres for Enhanced Optical Signal Amplification

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## Abstract

The optical properties of silica, essential for applications ranging from fibre optics to UV transmission windows, are closely linked to atomic-scale defects, even though they are challenging to identify. Although electron paramagnetic resonance (EPR) has long been the predominant technique for defect analysis, this study employs time-dependent density functional perturbation theory (TDDFPT) to systematically examine the understudied optical signatures of erbium (Er)-doped silica (SiO<sub>2</sub>) and native defects (oxygen/silicon vacancies). The Er-doped systems (2.08–6.25% concentrations) and pure SiO<sub>2</sub> along vacancy defects were simulated to compute transmittance, reflectivity, dielectric characteristics, and absorption. The results showed that the absorption peaks and imaginary dielectric function ( $\epsilon_2$ ) are redshifted by Er inclusion, with doping at 4.17% yielding the best improvement. Conversely, vacancy defects decrease otherwise because of increased absorption and reflection of the visible spectrum. These findings demonstrate how Er-doping can alter SiO<sub>2</sub>'s optical response and emphasize the value of TDDFPT in connecting optical behaviour to defect patterns. This study advances the logical design of silica-based optoelectronic devices and offers a theoretical foundation for enhancing defect engineering in wide-gap semiconductors.

Keywords: Silica; Erbium doping; Optical properties; TDDFPT; Defect engineering; Dielectric function.

## I. INTRODUCTION

The optical properties of silica are often one of the most important aspects of glassy applications [1]. They are reasonably easy to measure with standard spectrophotometers and offer instantaneous information on the quality of important silica-based devices, such as the attenuation of ultraviolet (UV) transmission windows [2] or fibre-optic waveguides [3]. However, optical measurements alone are

usually sufficient to determine the origin and atomic structure of the related point defects. The bulk of the information on the structures of defects in silica over the past few decades has come from electron paramagnetic resonance (EPR) studies since they are the most effective at "seeing" the atomic environment of the unpaired electron of a paramagnetic defect [4].

Due to EPR, optical spectroscopy has largely been overlooked in fundamental defect research. It was once thought that identifying a colour centre in silica involved two

steps: (i) figuring out the atomic structure of the defect using EPR, and (ii) figuring out which optical band, if any, coincides with the EPR signal. Only a small number of defect centres have demonstrated reliable correlations between the optical and EPR signals, and the second part of this study has proven to be quite difficult. Optical spectroscopy is particularly useful when EPR techniques are not appropriate, such as for diamagnetic defects, or when EPR optical correlations are distorted by inhomogeneous broadening effects [5].

Time-dependent density functional perturbation theory (TDDFPT) has recently been recognized as one of the most effective methods for accurately predicting optical properties within all defect centres [6]. As a result, many researchers have used TDDFPT to study how defects affect the optical properties of various wide-gap semiconductors [7], [8], yielding several results close to the experimental values for many applications. Lately, the focus of research has been on defects caused by Rare-earth (RE) doping in wide-gap semiconductors like silica, ZnO, etc. Reference [9] investigated the effects of an Er-defect on the optical characteristics of zinc oxide (ZnO) and discovered that Er-doped ZnO is an excellent dielectric material for high-frequency device applications. To our knowledge, a systematic investigation into the optical properties of defect states in silica has not yet been reported. In this study, we examine the effects of erbium-related defects on the optical behaviour of silica to advance the understanding of defect-induced optical modifications in this material.

## II. MODEL AND METHOD

### A. Model

As the primary material, we systematically modelled pure silica ( $\text{SiO}_2$ ), which has a tetragonal structure and is a member of the  $P4_2/mbc$  (135) space group. Its symmetry is  $4/mmm$ . In the unit cell, the structure is made up of 16 Si and 32 O atoms. The doping modelling was done by substituting one Si atom with one Er, which is equivalent to 2.08%, two Si atoms with

two Er, which is equivalent to 4.17%, and finally three Si atoms with three Er atoms, which is equivalent to 6.25% doping concentration. The effect of interstitial defects was further examined by removing one O atom from the optimized pure  $\text{SiO}_2$ , which is known as an oxygen vacancy defect ( $\text{O}_v$ ), and then removing another Si atom, which is known as a silicon vacancy defect ( $\text{Si}_v$ ).

### B. Computational Method

The optical characteristics of optoelectronic devices, such as light sources and detectors, are crucial to their designs and analyses. These characteristics are represented by the optical dielectric function. At all photon energies, the combined density of states and optical matrix elements are highly correlated with the imaginary component  $i\varepsilon_2(\omega)$  of the complex dielectric function by (1).

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (1)$$

Where  $\omega$  is the frequency,  $\varepsilon_1(\omega)$  is the real part, governing dispersion, and  $\varepsilon_2(\omega)$  is the imaginary part, related to absorption and loss. The actual portion  $\varepsilon_1(\omega)$  is obtained from  $i\varepsilon_2(\omega)$ . Both interband and intraband transitions affect  $\varepsilon(\omega)$ . In this study, the indirect interband transitions, which entail phonon scattering and are assumed to contribute marginally to  $\varepsilon(\omega)$  were neglected.

## III. RESULTS AND DISCUSSION

### A. Optical Absorption Coefficient

In Fig. 1(a), Er-doped  $\text{SiO}_2$  shows the black curve for pure  $\text{SiO}_2$ , which provides the baseline of these results. A first major absorption peak at  $\approx 12.5$  eV with an absorption coefficient of about  $2.5 \times 10^4 \text{ cm}^{-1}$  arises from O 2p nonbonding electrons excited into the Si 3p antibonding conduction band just above the fundamental gap (the 8.0 – 9.0 eV optical gap), and a second, stronger resonance at  $\approx 16.5$  eV ( $\approx 3.0 \times 10^4 \text{ cm}^{-1}$ ) originates from deeper O 2p bonding levels with excitonic enhancement into higher-lying Si 3d/4s conduction states [10], [11].

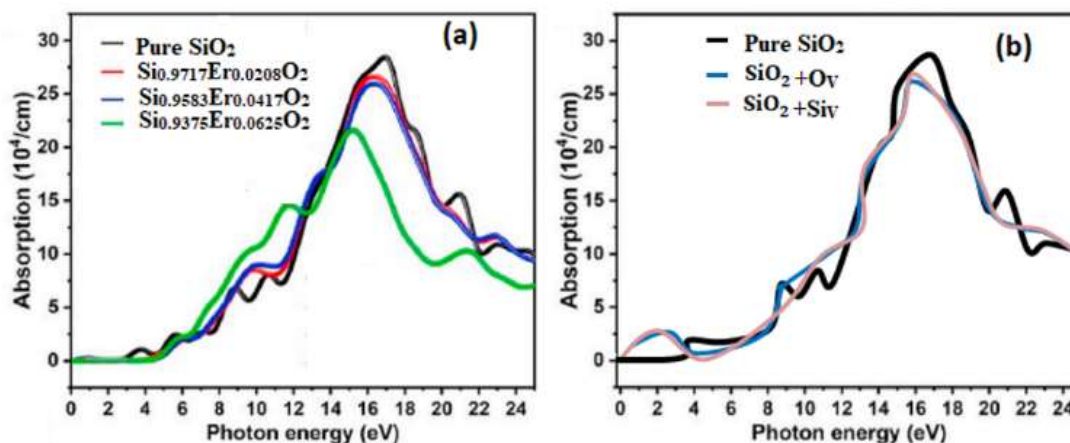


Fig. 1. Calculated optical absorption coefficient of (a) pure  $\text{SiO}_2$ ,  $\text{Si}_{0.9717}\text{Er}_{0.0283}\text{O}_2$ ,  $\text{Si}_{0.9583}\text{Er}_{0.0417}\text{O}_2$  and  $\text{Si}_{0.9375}\text{Er}_{0.0625}\text{O}_2$  (b) pure  $\text{SiO}_2$ ,  $\text{SiO}_2 + \text{O}_v$  and  $\text{SiO}_2 + \text{Si}_v$

Introducing  $\text{Er}^{3+}$  systematically perturbs these features; the red curve ( $x = 0.0208$ ) exhibits its main UV peak shifted down to  $\approx 12.3$  eV and reduced to  $\approx 2.4 \times 10^4 \text{ cm}^{-1}$ , indicating heavy  $\text{Er}^{3+}$  ions perturb the local Si–O network and mix Er 5d character into the conduction band [12]. Increasing the Er-doping concentration to  $x = 0.0417$  (blue curve) pushes that peak to  $\approx 12.2$  eV at  $2.3 \times 10^4 \text{ cm}^{-1}$ , while the secondary UV resonance near 16 eV likewise shifts and broadens [13]. At the highest Er concentration ( $x = 0.0625$ , green curve), the primary UV peak shifts to  $\approx 12.0$  eV with an intensity of only  $\approx 2.0 \times 10^4 \text{ cm}^{-1}$ , reflecting maximal lattice distortion and enhanced Er 4f–5d conduction-band hybridization that together lower the effective band-edge energy and diminish oscillator strength, thus producing a pronounced red shift and peak attenuation [14]. Across all doped curves, the gradual red shift and peak-height reduction illustrate how increasing Er concentration introduces intra-atomic 4f–5d transitions in the gap region (visible as faint shoulders near 3.0 – 5.0 eV) and perturbs the host's UV interband resonances [15], [16].

Fig. 1(b) compares pure  $\text{SiO}_2$  (black) with two intrinsic defect scenarios. In the defect-engineered samples, both the

oxygen-vacancy curve (blue) and the silicon-interstitial curve (brown) retain the two principal UV peaks near 12.0 – 17.0 eV but each is slightly broadened and red-shifted by  $\approx 0.1$  eV due to the disrupted Si–O network relative to pure  $\text{SiO}_2$ ; additionally, new sub-band-gap shoulders appear at 3.0 – 5.0 eV, marking optical transitions from defect-localized gap states into the conduction band, which give rise to visible-range absorption absent in pristine silica [17], [18]. For silicon interstitials (brown curve), mid-gap states produce a subgap absorption feature around 3.0 – 5.0 eV, while the UV peaks at  $\approx 12.3$  eV ( $\approx 2.3 \times 10^4 \text{ cm}^{-2}$ ) and  $\approx 16.4$  eV ( $\approx 2.7 \times 10^4 \text{ cm}^{-1}$ ) are again slightly red-shifted and broadened relative to pure  $\text{SiO}_2$  [19]. Together, these defect curves show that network disruptions, whether by missing oxygen or extra silicon create localized electronic levels inside the fundamental gap that absorb visible photons and simultaneously perturb the high-energy interband and excitonic resonances inherited from the O 2p  $\rightarrow$  Si 3p/3d transitions of the undisturbed matrix. The calculated optical absorption coefficient peak characteristics variations are shown in Table I.

Table I. Calculated optical absorption coefficient peak characteristics variations.

| Material                                         | Peak Energy (eV) | Peak Intensity ( $10^4 \text{ cm}^{-1}$ ) | Peak Shape      | Likely Cause                                  |
|--------------------------------------------------|------------------|-------------------------------------------|-----------------|-----------------------------------------------|
| Pure $\text{SiO}_2$                              | 13.0 – 14.0      | 25.0 – 27.0                               | Broad           | Interband transitions.                        |
| $\text{Si}_{0.9717}\text{Er}_{0.0208}\text{O}_2$ | 13.0             | 22.0 – 24.0                               | Broad           | induced additional states.                    |
| $\text{Si}_{0.9583}\text{Er}_{0.0417}\text{O}_2$ | 13.0 – 14.0      | 27.0 – 28.0                               | Broad, intense  | Higher Er doping enhances absorption.         |
| $\text{SiO}_2 + \text{O}_v$                      | 13.0             | 27.0 – 28.0                               | Sharp, intense  | $\text{O}_v$ states near the conduction band. |
| $\text{SiO}_2 + \text{Si}_v$                     | 13.0 – 14.0      | 25.0 – 26.0                               | Broad, shoulder | $\text{Si}_v$ states near the valence band.   |

### B. Optical Transmittance Coefficient

Fig. 2(a) illustrates the optical transmittance of pure  $\text{SiO}_2$  and  $\text{SiO}_2$  doped with erbium (Er) at concentrations of 4.17% ( $\text{Si}_{0.9583}\text{Er}_{0.0417}\text{O}_2$ ), 6.25% ( $\text{Si}_{0.9375}\text{Er}_{0.0625}\text{O}_2$ ), and 12.5% ( $\text{Si}_{0.9717}\text{Er}_{0.0208}\text{O}_2$ ). The pure  $\text{SiO}_2$  (black curve) exhibits a peak transmittance of  $\sim 85\%$  at  $\sim 3.0$  eV ( $\sim 413$  nm) and falls below 20% by 12.0 eV ( $\sim 103$  nm), reflecting its intrinsic band-edge absorption [20]. At 12.5% Er, the peak transmittance decreases to 60% at 3.0 eV with a pronounced red shift, and transmittance plunges below 5% at 12.0 eV due to additional  $\text{Er}^{3+}$ -related absorption centres [21]. In the 2.08% Er sample (red curve), transmittance remains high in the visible (1.65 – 3.1 eV), peaking at 85% at 3 eV, then decreases sharply, falling below 20% at 12.0 eV and approaching 0% at 20.0 eV; this behaviour is typical of low-concentration  $\text{Er}^{3+}$ -doped silica produced via sol–gel processes [22], and is governed by Er 4f–4f and charge-transfer transitions [23]. At 4.17% Er (blue curve), the visible-range peak is  $\sim 75\%$  at 3.0 eV with UV transparency enhanced: transmittance rises to  $\sim 30\%$  between 12.0 – 14.0 eV compared to near-zero in undoped  $\text{SiO}_2$ , suggesting that moderate Er doping passivates native

defects (e.g. non-bridging oxygen-hole centres and E' centres), reducing UV absorption [24], [25]. With 6.25% Er (green curve), peak transmittance falls to 70% at 3.0 eV and declines to 10% by 12.0 eV, indicating that higher Er concentrations introduce a greater density of localized electronic states within the bandgap that enhance visible-range absorption [26]. The trend of decreasing peak transmittance ( $85\% \rightarrow 75\% \rightarrow 70\% \rightarrow 60\%$ ) and red shifting with increased Er content is consistent with the progressive introduction of electronic defect states by  $\text{Er}^{3+}$  ions [27].

Fig. 2(b) compares pure  $\text{SiO}_2$  with oxygen-vacancy ( $\text{SiO}_2 + \text{O}_v$ , yellow curve) and silicon-vacancy ( $\text{SiO}_2 + \text{Si}_v$ , cyan curve) samples. Oxygen vacancies reduce the peak transmittance to  $\sim 60\%$  at 3.0 eV and produce a rapid drop to 10% by 10.0 eV, approaching 0% by 18.0 eV, showing that  $\text{O}_v$  acts as strong absorption/scattering centres [28]. Silicon vacancies have an even stronger effect, lowering the peak to  $\sim 50\%$  at 3.0 eV and causing transmittance to fall below 5% by 10.0 eV, due to deep-level traps and significant lattice disruption [29], [30]. Both  $\text{O}_v$  and  $\text{Si}_v$  substantially diminish  $\text{SiO}_2$ 's transmission, with  $\text{Si}_v$  having the more pronounced

impact (50% vs 60% peak transmittance). The steeper declines and spectral fluctuations between 6.0 – 12.0 eV indicate the creation of midgap states that increase absorption

across the UV–Vis range [31]. The Optical Transmittance Peaks with key observations are depicted in Table II.

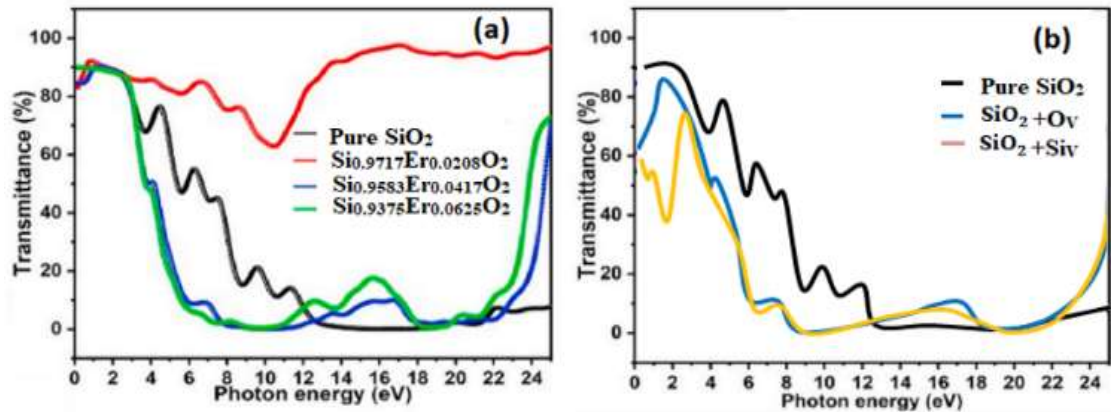


Fig. 2. Transmittance Coefficient of (a) pure SiO<sub>2</sub>, Si<sub>0.9717</sub>Er<sub>0.0208</sub>O<sub>2</sub>, Si<sub>0.9583</sub>Er<sub>0.0417</sub>O<sub>2</sub> and Si<sub>0.9375</sub>Er<sub>0.0625</sub>O<sub>2</sub> (b) pure SiO<sub>2</sub>, SiO<sub>2</sub> + O<sub>v</sub> and SiO<sub>2</sub> + Si<sub>v</sub>

Table II. Optical Transmittance Peaks.

| Sample                                                   | Colour in Fig. 2 | Peak Transmittance (%T) | Photon Energy at Peak (eV) | Region      | Key Observation                               |
|----------------------------------------------------------|------------------|-------------------------|----------------------------|-------------|-----------------------------------------------|
| Pure SiO <sub>2</sub> (a)                                | Red              | 85.0                    | 3.0                        | Visible     | High transparency in the visible range.       |
| Si <sub>0.9583</sub> Er <sub>0.0417</sub> O <sub>2</sub> | Blue             | 75.0 (30.0 in UV)       | 3.0 (12 – 14 in UV)        | Visible, UV | Increased UV transmittance at 4.17% Er.       |
| Si <sub>0.9375</sub> Er <sub>0.0625</sub> O <sub>2</sub> | Green            | 70.0                    | 3.0                        | Visible     | Decreased transmittance, slight red shift.    |
| Si <sub>0.875</sub> Er <sub>0.125</sub> O <sub>2</sub>   | Black            | 60.0                    | 3.0                        | Visible     | Further decrease, pronounced red shift.       |
| Pure SiO <sub>2</sub> (b)                                | Black            | 85.0                    | 3.0                        | Visible     | Baseline high transmittance.                  |
| SiO <sub>2</sub> + O <sub>v</sub>                        | Yellow           | 60.0                    | 3.0                        | Visible     | Reduced transmittance due to O <sub>v</sub> . |
| SiO <sub>2</sub> + Si <sub>v</sub>                       | Cyan             | 50.0                    | 3.0                        | Visible     | Strongest reduction due to Si <sub>v</sub> .  |

C. Dielectric function

Fig. 3 presents the imaginary part of the dielectric function ( $\epsilon_2$ ) for various silica-based materials, offering a window into their dielectric and optical properties across the energy range of 0 to 24.0 eV [32]. The dielectric function, a complex quantity expressed in (1), describes how the material interacts with electromagnetic radiation [33]. The imaginary part,  $\epsilon_2$ , specifically relates to energy dissipation and absorption [34], while the real part,  $\epsilon_1$ , is associated with polarization and refraction [35]. Since Fig. 3 focuses on  $\epsilon_2$ , the dielectric properties were delved into, exploring the implications of the observed peaks, such as the effects of erbium doping and non-stoichiometric modifications, and their broader significance for optical and electronic applications. This analysis also ties these observations to the relationships between  $\epsilon_2$  and other

optical parameters, such as the extinction coefficient, absorption coefficient, and reflectivity [36]. The dielectric function quantifies a material's response to an electric field, such as incident light. The imaginary part,  $\epsilon_2$ , is directly proportional to the material's ability to absorb energy from the electromagnetic wave, reflecting processes like interband transitions, excitonic effects, or defect-related absorption [37]. Peaks in  $\epsilon_2$  indicate energies where these absorption processes are most pronounced and manifest as critical points in the joint density of states [38].

Fig. 3(a) compares pure SiO<sub>2</sub> (black), Si<sub>0.9717</sub>Er<sub>0.0208</sub>O<sub>2</sub> (red), Si<sub>0.9583</sub>Er<sub>0.0417</sub>O<sub>2</sub> (blue), and Si<sub>0.9375</sub>Er<sub>0.0625</sub>O<sub>2</sub> (green), showing the effect of increasing erbium doping. Fig. 3(b) compares pure SiO<sub>2</sub> (black), SiO<sub>2</sub> + O<sub>v</sub> (blue), and SiO<sub>2</sub> + Si<sub>v</sub> (yellow), illustrating the impact of oxygen and silicon excess. The

energy range of 0 – 24.0 eV corresponds to the ultraviolet (UV) and vacuum-UV spectrum, where silica-based materials typically exhibit strong absorption due to their wide bandgap (~9.0 eV) [39] and multiple interband transitions [40]. The dielectric properties inferred from  $\epsilon_2$  are critical for applications such as optical coatings, waveguides, dielectric layers in electronics, and UV optics, where controlling absorption, refraction, and energy dissipation is essential [41]. Fig. 3(a) shows how erbium doping alters the dielectric properties of silica, as evidenced by changes in the magnitude and shape of  $\epsilon_2$  peaks. The pure  $\text{SiO}_2$  (black curve) exhibits a primary peak at 10.0 – 12.0 eV (~10.4 eV, 11.6 eV) corresponding to the fundamental interband transitions near the bandgap edge, with an intensity of ~1.0 – 1.2 [42]. A secondary peak at 18.0 – 20.0 eV (e.g., 16.2 eV, 20.1 eV) arises from higher-energy core-electron resonances and plasmonic features [43]. In dielectric terms, these features indicate additional energy-dissipation channels at higher photon energies, though less dominant than the bandgap absorption. Er-doping (red, blue, green curves) systematically increases the intensity of both the primary (to ~1.5 – 3.0) and

secondary (to ~0.8–1.5)  $\epsilon_2$  peaks, reflecting the introduction of erbium-related electronic states that enhance absorption and dielectric loss in the UV [44].  $\text{Si}_{0.9717}\text{Er}_{0.0283}\text{O}_2$  shows moderate enhancement (primary ~1.5 – 1.8; secondary ~0.8–1.0),  $\text{Si}_{0.9583}\text{Er}_{0.0417}\text{O}_2$  stronger (primary ~2.0 – 2.5; secondary ~1.0 – 1.2), and  $\text{Si}_{0.9375}\text{Er}_{0.0625}\text{O}_2$  the most pronounced (primary ~2.5 – 3.0; secondary ~1.2 – 1.5). This trend implies an increasing density of erbium-related defect or impurity states that facilitate UV absorption, which can be exploited in applications like UV filters, sensors, or photonic devices requiring controlled absorption [45].

Fig. 3(b) illustrates that oxygen vacancies ( $\text{SiO}_2 + \text{O}_v$ ) introduce sub-bandgap absorption features (e.g., around 7.6 eV) due to defect-level transitions [46], while silicon excess ( $\text{SiO}_2 + \text{Si}_v$ ) similarly modifies the UV absorption profile through Si-related dangling-bond states. These defect-induced absorption bands broaden  $\epsilon_2$  and increase dielectric loss, impacting the transparency and performance of  $\text{SiO}_2$  dielectrics in UV-critical applications [47]. The dielectric properties based on  $\epsilon_2$  peaks are presented in Table III.

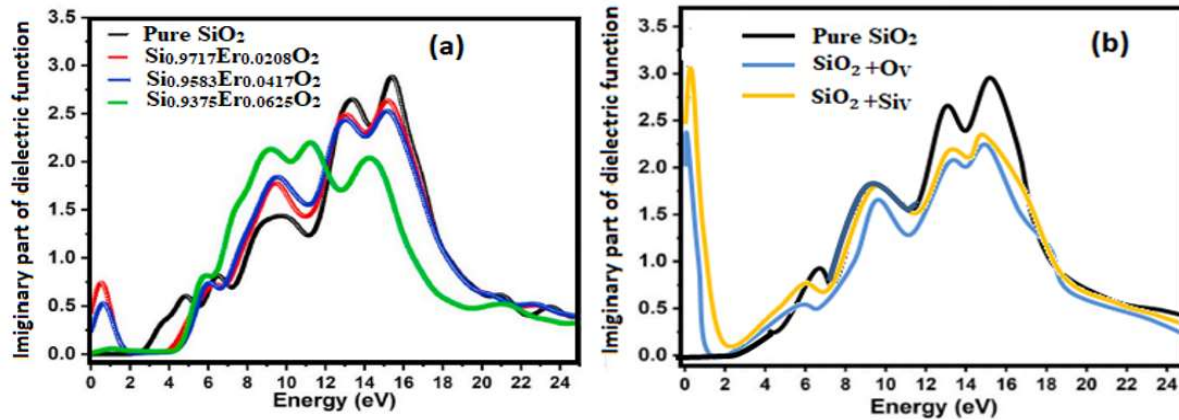


Fig. 3. The imaginary part of the dielectric function of (a) pure  $\text{SiO}_2$ ,  $\text{Si}_{0.9717}\text{Er}_{0.0283}\text{O}_2$ , and  $\text{Si}_{0.9583}\text{Er}_{0.0417}\text{O}_2$ , and  $\text{Si}_{0.9375}\text{Er}_{0.0625}\text{O}_2$  (b)  $\text{SiO}_2 + \text{O}_v$  and  $\text{SiO}_2 + \text{Si}_v$

Table III. Dielectric Properties Based on  $\epsilon_2$  Peaks.

| Material                                         | Colour in Fig. 3 | Primary Peak (eV) | Primary Peak Intensity | Secondary Peak (eV) | Secondary Peak Intensity | Dielectric Loss Implication                      |
|--------------------------------------------------|------------------|-------------------|------------------------|---------------------|--------------------------|--------------------------------------------------|
| Pure $\text{SiO}_2$                              | Black            | 10.0-12.0         | 1.0-1.2                | 18.0-20.0           | 0.5-0.7                  | Low loss, suitable for low-loss dielectrics.     |
| $\text{Si}_{0.9717}\text{Er}_{0.0283}\text{O}_2$ | Red              | 10.0-12.0         | 1.5-1.8                | 18.0-20.0           | 0.8-1.0                  | Moderate loss, increased absorption.             |
| $\text{Si}_{0.9583}\text{Er}_{0.0417}\text{O}_2$ | Green            | 10.0-12.0         | 2.0-2.5                | 18.0-20.0           | 1.0-1.2                  | Higher loss, stronger absorption.                |
| $\text{Si}_{0.9375}\text{Er}_{0.0625}\text{O}_2$ | Blue             | 10.0-12.0         | 2.5-3.0                | 18.0-20.0           | 1.2-1.5                  | Highest loss in Fig. 3(a), strongest absorption. |
| $\text{SiO}_2 + \text{O}_v$                      | Blue             | 8.0-10.0          | 2.0-2.5                | 18.0-20.0           | 0.8-1.0                  | High loss, shifted absorption due to defects.    |
| $\text{SiO}_2 + \text{Si}_v$                     | Yellow           | 8.0-10.0          | 2.5-3.0                | 18.0-20.0           | 1.0-1.2                  | Highest loss in Fig.3(b), strongest absorption.  |

#### D. Reflectivity coefficient

Fig. 4(a) presents the reflectivity of pure  $\text{SiO}_2$  and Er-doped  $\text{SiO}_2$  as a function of photon energy, with each sample represented by a distinct colour to facilitate comparison [48]. The reflectivity curves reveal how erbium doping modifies the optical properties of  $\text{SiO}_2$ , particularly in the UV range [49]. The Pure  $\text{SiO}_2$  (Black Curve) shows a gradual increase in reflectivity with increasing photon energy. It reaches a peak reflectivity of approximately 0.15 (15%) around 20.0 – 22.0 eV, indicating that 15% of the incident light is reflected at these high energies in the UV region. This relatively low reflectivity underscores  $\text{SiO}_2$ 's transparency in the visible range and moderate reflectivity in the UV range, consistent with its use in optical applications [50]. In the  $\text{Si}_{0.9717}\text{Er}_{0.0208}\text{O}_2$  (2.0% Er, Red Curve), the reflectivity increases more rapidly than in pure  $\text{SiO}_2$ , peaking at approximately 0.20 (20 %) around 18.0 – 20.0 eV [51]. This enhancement suggests that even a small amount of Er doping introduces electronic states

that increase light reflection, particularly in the UV region [52]. The slight shift in peak energy compared to pure  $\text{SiO}_2$  indicates a modification in the material's band structure. For the  $\text{Si}_{0.9583}\text{Er}_{0.0417}\text{O}_2$  (4.1% Er, Blue Curve), at a higher Er concentration of 4.1%, the peak reflectivity rises to 0.22 (22%) at 18 eV. The peak is sharper and more pronounced than in the 2.0% Er sample, reflecting a stronger influence of erbium on the material's optical properties. This increase in reflectivity suggests that additional Er ions create more defect-related energy levels, enhancing light scattering or reflection [53]. Finally, in the  $\text{Si}_{0.9375}\text{Er}_{0.0625}\text{O}_2$  (6.2% Er, Green Curve), the reflectivity reaches its maximum at 0.25 (25%) at 18.0 eV, the highest among all samples. This peak is not only higher but also occurs at well-defined energy, indicating that higher Er doping significantly alters the electronic structure of  $\text{SiO}_2$ , leading to increased reflectivity in the UV range. The Reflectivity Coefficient Peaks of the samples are shown in Table IV.

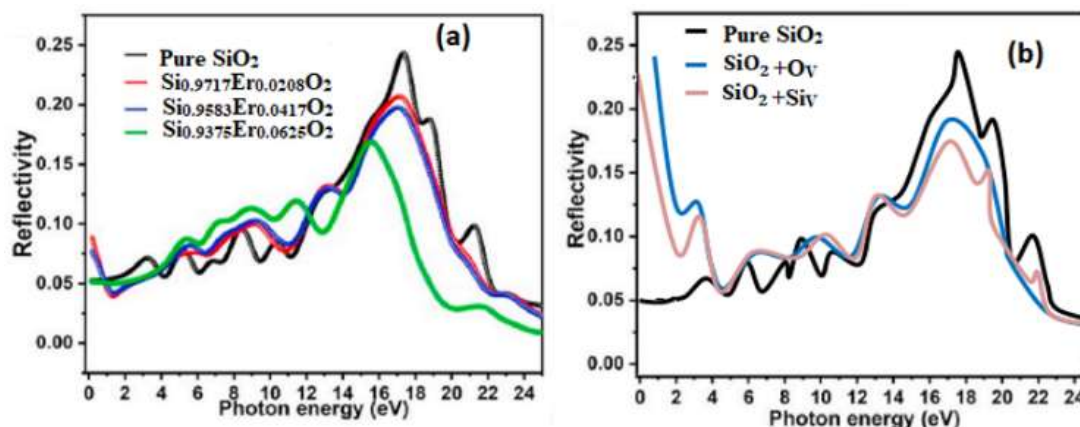


Fig. 4. Reflectivity coefficient of (a) pure  $\text{SiO}_2$ ,  $\text{Si}_{0.9717}\text{Er}_{0.0208}\text{O}_2$ ,  $\text{Si}_{0.9583}\text{Er}_{0.0417}\text{O}_2$  and  $\text{Si}_{0.9375}\text{Er}_{0.0625}\text{O}_2$  (b) pure  $\text{SiO}_2$ ,  $\text{SiO}_2 + \text{O}_v$  and  $\text{SiO}_2 + \text{Si}_v$ .

Table IV. Reflection Coefficient Peaks.

| Sample                                                      | Colour in Fig. 4 | Peak Reflectivity | Photon Energy at Peak (eV) | Region |
|-------------------------------------------------------------|------------------|-------------------|----------------------------|--------|
| Pure $\text{SiO}_2$ (a, b)                                  | Black            | 0.15              | 20.0–22.0                  | UV     |
| $\text{Si}_{0.971}\text{Er}_{0.0208}\text{SiO}_2$ (2.0% Er) | Red              | 0.20              | 18.0–20.0                  | UV     |
| $\text{Si}_{0.953}\text{Er}_{0.041}\text{SiO}_2$ (4.1% Er)  | Green            | 0.22              | 18.0                       | UV     |
| $\text{Si}_{0.937}\text{Er}_{0.062}\text{SiO}_2$ (6.2% Er)  | Blue             | 0.25              | 18.0                       | UV     |
| $\text{SiO}_2 + \text{O}_v$                                 | Blue             | 0.20              | 18.0                       | UV     |
| $\text{SiO}_2 + \text{Si}_v$                                | Pink             | 0.22              | 18.0                       | UV     |

Fig. 4(b) shows the impact of native defects, oxygen vacancies ( $\text{O}_v$ ) and silicon vacancies ( $\text{Si}_v$ ), on the reflectivity of  $\text{SiO}_2$  [53]. These defects introduce structural and electronic changes that alter the material's optical properties, with each sample represented by a distinct colour. The Pure  $\text{SiO}_2$  (Black Curve), consistent with Fig. 4 (a), serves as the reference, peaking at 0.15 (15%) around 20.0 – 22.0 eV. This baseline reflectivity reflects the intrinsic optical properties of  $\text{SiO}_2$ ,

with moderate reflection in the UV range and high transparency in the visible spectrum [54]. The  $\text{SiO}_2 + \text{O}_v$  (Blue Curve) shows that the introduction of oxygen vacancies increases the reflectivity, with a peak of approximately 0.20 (20%) at 18.0 eV. This enhancement indicates that  $\text{O}_v$  creates defect states within the band gap that increase light scattering or reflection, particularly in the UV range [55]. The peak at 18.0 eV suggests a shift in the optical response compared to

pure SiO<sub>2</sub>, similar to the effect observed with Er doping. In contrast, the SiO<sub>2</sub> + Si<sub>v</sub> (Pink Curve) shows that silicon vacancies have a more significant impact, with a peak reflectivity of 0.22 (22%) at 18.0 eV [56]. The curve for SiO<sub>2</sub> + Si<sub>v</sub> is sharper than that for SiO<sub>2</sub> + O<sub>v</sub>, indicating a more localized effect on the material's optical properties [57]. The rapid decline after the peak suggests that Si<sub>v</sub> introduces deep donor levels that enhance reflectivity within a narrow energy range, particularly in the UV region.

#### IV. CONCLUSION

The combined optical and dielectric analyses show that both erbium doping and intrinsic defect offer strong ways to customise the UV-visible response of silica. The incorporation of Er<sup>3+</sup> attenuates and redshifts the primary interband absorption peaks (from  $\approx 12.5$  eV to  $\approx 12.0$  eV) while introducing weaker intra-4f–5d resonances in the 3 – 5 eV range. In turn, transmittance in the visible decreases (85% to 60% at 3 eV) as Er concentration increases, while dielectric loss ( $\epsilon_2$ ) and reflectivity in the UV both rises, reflecting improved absorption channels and altered band-edge structure. The Si–O network is similarly perturbed by silicon interstitials and oxygen vacancies: each defect species produces sub-bandgap shoulders around 3 – 5 eV, increases dielectric loss and reflectivity at 18 eV, and redshifts and broadens the  $\approx 12$  – 17 eV UV resonances by  $\sim 0.1$  eV. The unique electronic fingerprints of various defect types are highlighted by the significantly higher midgap absorption and reflectivity enhancement exerted by silicon interstitials compared to oxygen vacancies. These findings, together measure the extent to which silica's optical edge, absorption strength, and dielectric behaviour may be engineered using rare-earth doping and regulated defect populations. Such tunability benefits the design of UV-optical coatings, photonic devices, and dielectric layers, where precise control of band-edge absorption, transmittance, and energy dissipation is essential.

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