

Supporting information.

Defect passivation in (Er³⁺/Nd³⁺) codoped TiO₂ photoanode and its application towards enhanced solar energy conversion devices

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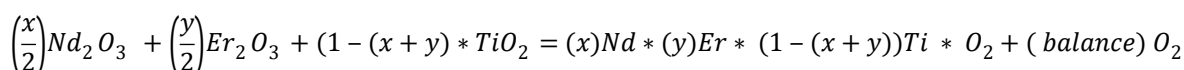
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S1. stoichiometry calculations of RE Co-dopants with TiO₂



$$\Rightarrow \left(\frac{x}{2}\right)\left(336.48\frac{g}{mol}\right) + \left(\frac{y}{2}\right)\left(382.56\frac{g}{mol}\right) + (1 - (x + y)) * \left(79.87\frac{g}{mol}\right)$$

$$= x (144.2) * y (167.2) * (1 - (x + y))\left(47.87\frac{g}{mol}\right) * 32 + (balance) 32$$

For 1gram amount of powder

$$\Rightarrow Nd_2O_3 \text{ concentration} = \frac{\left(\frac{x}{2}\right)\left(336.48\frac{g}{mol}\right)}{x (144.2) * y (167.2) * (1 - (x + y))\left(47.87\frac{g}{mol}\right) * 32}$$

$$\Rightarrow \text{Er}_2\text{O}_3 \text{ concentration} = \frac{\left(\frac{x}{2}\right)\left(382.56 \frac{\text{g}}{\text{mol}}\right)}{x(144.2) * y(167.2) * (1 - (x + y))\left(47.87 \frac{\text{g}}{\text{mol}}\right) * 32}$$

$$\Rightarrow \text{TiO}_2 \text{ concentration} = \frac{(1 - x) * \left(79.87 \frac{\text{g}}{\text{mol}}\right)}{x(144.2) * y(167.2) * (1 - (x + y))\left(47.87 \frac{\text{g}}{\text{mol}}\right) * 32}$$

S2. W-H plots

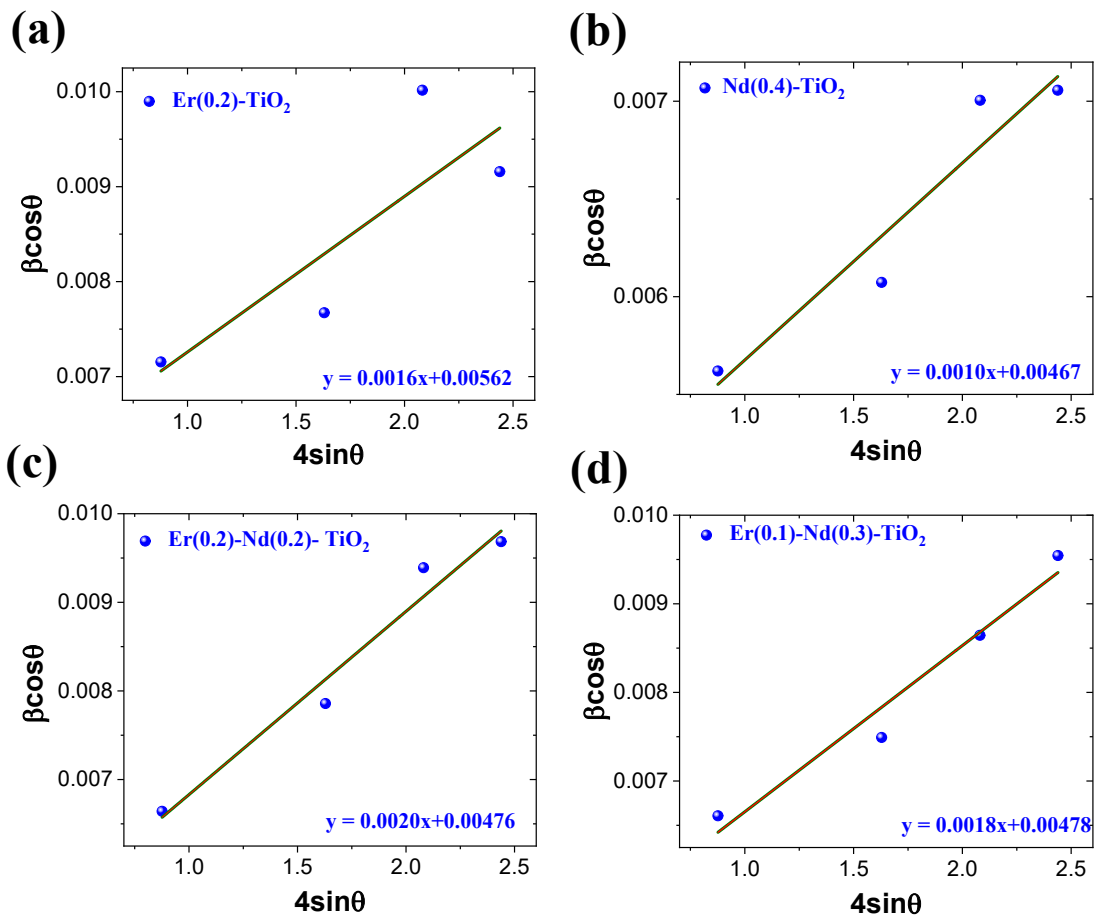


Figure S1(a-d). grain size and stress calculation by W-H method

S3. UV diffused reflectance spectrum

Er³⁺ doped TiO₂ bandgap is found to be increased with respective Er-doping concentrations of 0.1%, 0.3% and 0.4%, as I reported in my previous work¹. Nd³⁺ doped TiO₂ band gap is observed to be reduced with respective Nd doping concentrations of 0.2%, 0.3%, and 0.5% mol as I reported in my previous work².

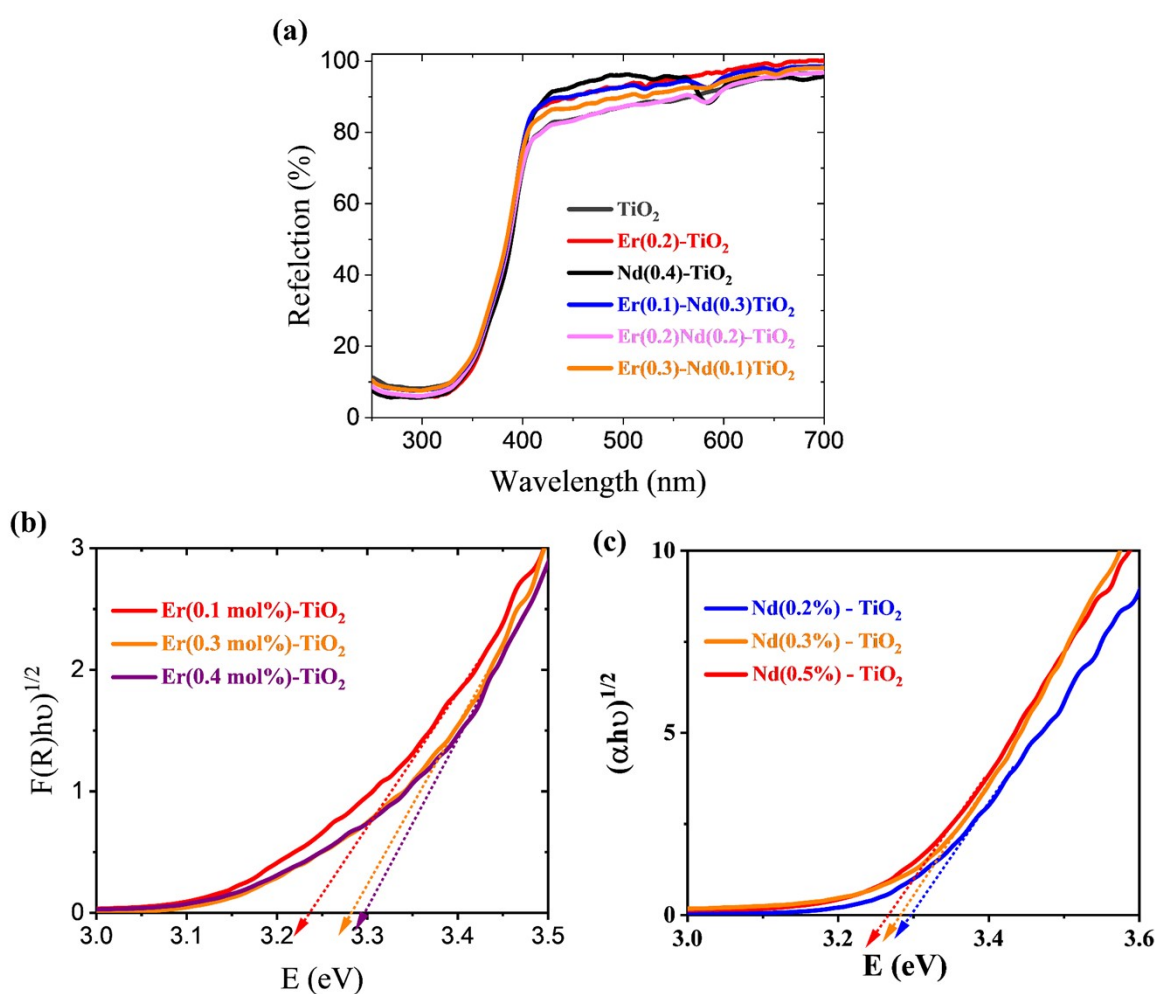


Figure S2. (a) DRS reflectance spectrum; (b-c) bandgap of Er doping series of (0.1%, 0.2%, 0.3, and 0.4% mol), and Nd doping series (0.2%, 0.3%, and 0.5% mol)

S4. PEC Results

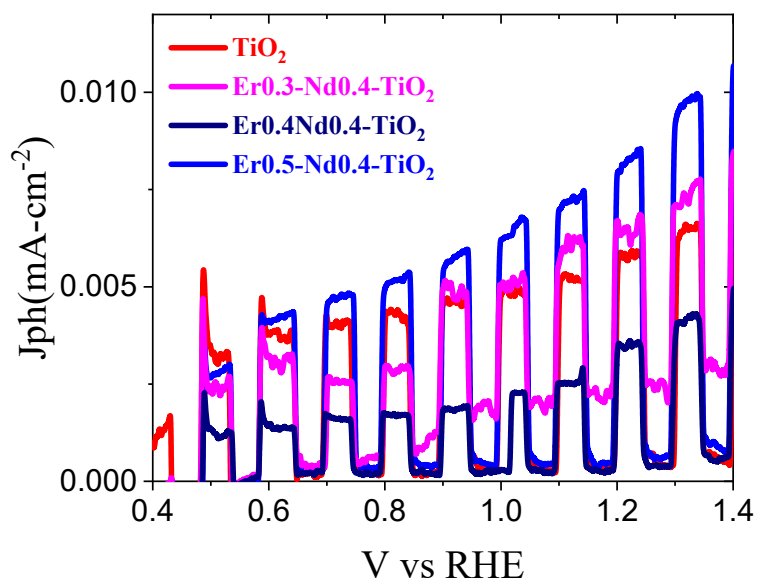


Figure S3. Linear sweep voltammetry of PEC water splitting with neutral Na_2SO_4 electrolyte.

S5. Experimental details

S5.1. CdS layer deposition

The successive ionic layer deposition (SILAR) technique has been extensively used to fabricate homogeneous quantum dots. Preparation of the controllable-sized CdS quantum dot manufacturing is extremely effective. In this approach, TiO_2 coated films are dipped for two minutes in a cationic solution of (0.1 M $\text{Cd}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$, dissolved in ethanol) and washed in ethanol to remove any remaining unabsorbed ions, followed by a two-minute heat treatment at 70°C. The same films were dipped for 2 minutes in an anionic solution (0.1 M Na_2S dissolved in ethanol), washed in ethanol to remove unabsorbed salts, and then thermalized for 2 minutes at 70°C. It is regarded as a single cycle of QDs deposition using the SILAR technique. Similarly, six further cycles were performed to determine the ideal size QDs for the TiO_2 photoanode³.

S5.2. N719 ruthenium dye loading

0.3 millimoles Ruthenium N719 dye and acetonitrile (ACN) were utilised to produce monolayer dyes on TiO_2 coated substrates. The films were immersed in a solution of ruthenium. Following dye loading for 24 hours, the samples were washed in acetonitrile to eliminate any remaining dye molecules.

1. V. S. Katta, M. Velpandian, V. R. Chappidi, M. S. Ahmed, A. Kumar, S. Asthana, P. Meduri and S. S. K. Raavi, *Materials Letters*, 2021, 130297.
2. V. S. Katta, A. Das, G. Cilaveni, S. Pulipaka, G. Veerappan, E. Ramasamy, P. Meduri, S. Asthana, D. Melepurath and S. S. K. Raavi, *Solar Energy Materials and Solar Cells*, 2021, **220**, 110843.
3. P. Subramanyam, P. N. Kumar, M. Deepa, C. Subrahmanyam and P. Ghosal, *Solar Energy Materials and Solar Cells*, 2017, **159**, 296-306.