

Synthesis and photocatalytic performance of yttrium-doped CeO₂ with a porous broom-like hierarchical structure

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| 著者 | Xu Bin, Zhang Qitao, Yuan Saisai, Zhang Ming, Ohno Teruhisa |
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Table.1: Rietveld refined data from XRD patterns and oxygen vacancy value calculated by Raman spectra.

| Samples/ different mole ratio | Lattice parameters (a) | Calculated grain size (nm) | R _{wp} | Particles size (nm) | Area _{Oxygen vacancies} /Area _{F2g} (%) |
|-------------------------------------|---------------------------|-------------------------------|-----------------|---------------------------|--|
| Pure CeO ₂ | 5.4178 | 4.50 | 5.86 | ~10 | 6.8 |
| 1 : 0.05 | 5.4190 | 4.6 | 5.26 | ~10 | 10.9 |
| 1 : 0.1 | 5.4240 | 4.52 | 5.76 | ~10 | 11.2 |
| 1 : 0.2 | 5.4228 | 4.54 | 5.05 | ~10 | 10.2 |
| 1 : 0.3 | 5.4249 | 4.6 | 4.87 | ~10 | 10.5 |
| 1 : 0.4 | 5.4273 | 4.63 | 5.62 | ~10 | 10.3 |

PS: $\text{Area}_{\text{Oxygen vacancies}} / \text{Area}_{\text{F2g}} (\%) = (\text{Area}_{\text{Rdoped}} + \text{Area}_{\text{Rce-o}}) / \text{Area}_{\text{Fag}} (\%)$

Table.2: Calculated [Ce³⁺] and [O_{sur}] concentrations of as-fabricated samples from the XPS spectrum.

| Sample/different mole ratio of Ce and Y | [Ce ³⁺]/[Ce ³⁺ +Ce ⁴⁺] % | [O _{sur}]/[O _{sur} +O _{lat}] % |
|---|---|---|
| Pure CeO ₂ | 19.0 | 40.5 |
| 1: 0.05 | 25.38 | 52.8 |
| 1: 0.1 | 29.76 | 55.8 |
| 1: 0.2 | 23.43 | 52.76 |
| 1: 0.3 | 24.00 | 53.59 |
| 1: 0.4 | 23.86 | 53.97 |

$$\frac{[\text{Ce}^{3+}]}{[\text{Ce}^{3+} + \text{Ce}^{4+}]} = \frac{\text{area}(V_0, V_1, U_0, U_1)}{\text{total area}}$$

$$\frac{[\text{O}_{\text{sur}}]}{[\text{O}_{\text{sur}} + \text{O}_{\text{lat}}]} = \frac{\text{area}(\text{O}_{\text{sur}})}{\text{total area}}$$