Supporting information

Polymorphic phase study on Nitrogen-doped TiO_2 nanoparticles: Effect on oxygen site occupancy, dye sensitized solar cells efficiency and hydrogen production

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In order to calculate the percentage of anatase and rutile phase in the samples, in addition to the concentration of defects, we have obtained XRD spectra of the samples and by Rietveld Refinement using Anatase (JCPDS # 84-1286; CIF # 20-2243) and Rutile (JCPDS # 76-0649; CIF # 34-372) the diffraction profile was built.

The fitting was performed according to the following sequence:

Scale factor, zero point of detector, background (using linear interpolation), lattice parameters, atomic positions, overall Debye-Waller factor anisotropic, peak shape and asymmetry parameters, atom occupancies, finally microstructural parameters: size (using harmonics spherical corrections) and strain effects.

In a mixture of N crystalline phases the weight fraction W_j of phase is given by:

$$W_j = \frac{S_j Z_j M_j V_j / t_j}{\sum S_i Z_i M_i V_i / t_i}$$

where S_j is the scale factor of phase j, Z_j is the number of formula units per unit cell for phase j, M_j is the mass of the formula unit, V_j is the unit cell volume, t_j is the Brindley particle absorption contrast factor for phase j.

The crystallographic structure factor F_j is calculated in FULLPROF by using formula:

$$F_h = \sum_{j=1}^{n} O_j f_j(h) exp\left(-B_j(h)/4\right) \sum_{s=1}^{m} T_{js}(h) exp2pii(h^T S_s rj + h^T t_s)$$

where n is the number of atoms in the asymmetric unit, m is the number of the reduced set of symmetry operators. O_j is the occupation factor, $f_j(h)$is the scattering length, $B_j$is the isotropic temperature parameter, $r_j$is the position vector of atom j.