

Supporting Information

Cd-ZnGeON solid solution: effect of local electronic environment on their photocatalytic ability of water cleavage

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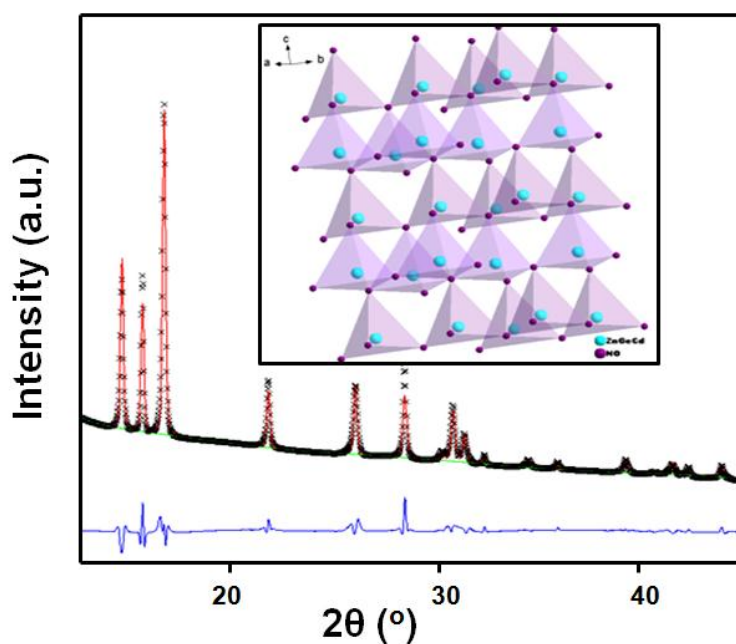


Figure S1 Experimental (crosses), calculated (solid line), and difference (bottom) results of SR-XRD refinement of wurtzite Cd-ZnGeON sample (nitrided at 800°C), crystallise in a centric primitive hexagonal phase with space group $P6_3mC$ and their reliability factors $\chi^2=2.958$, $R_{wp}=0.051$, $R_p=0.0318$ and $R(f^2)=0.2337$ within a permissible limit. Inset contains a schematic crystal structure of five unit cells, revealing a well ordered array of the CdZnGe (blue) and ON (purple) that arranged in a tetrahedral fashion.

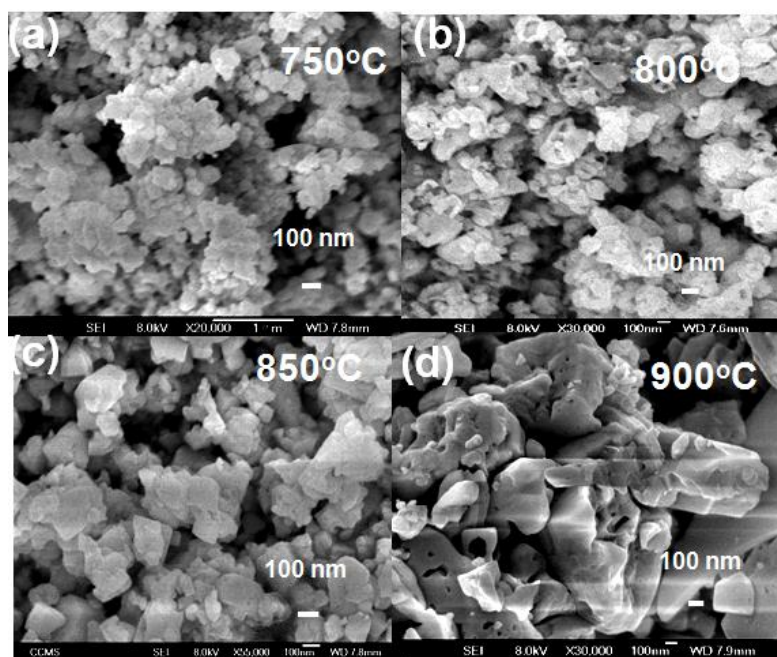


Figure S2 SEM micrographs of solid solution Cd-ZnGeON synthesised at (a) 750°C, (b) 800°C, (c) 850°C and (d) 900°C, where, 1-bar symbol represents 100nm of particle size.

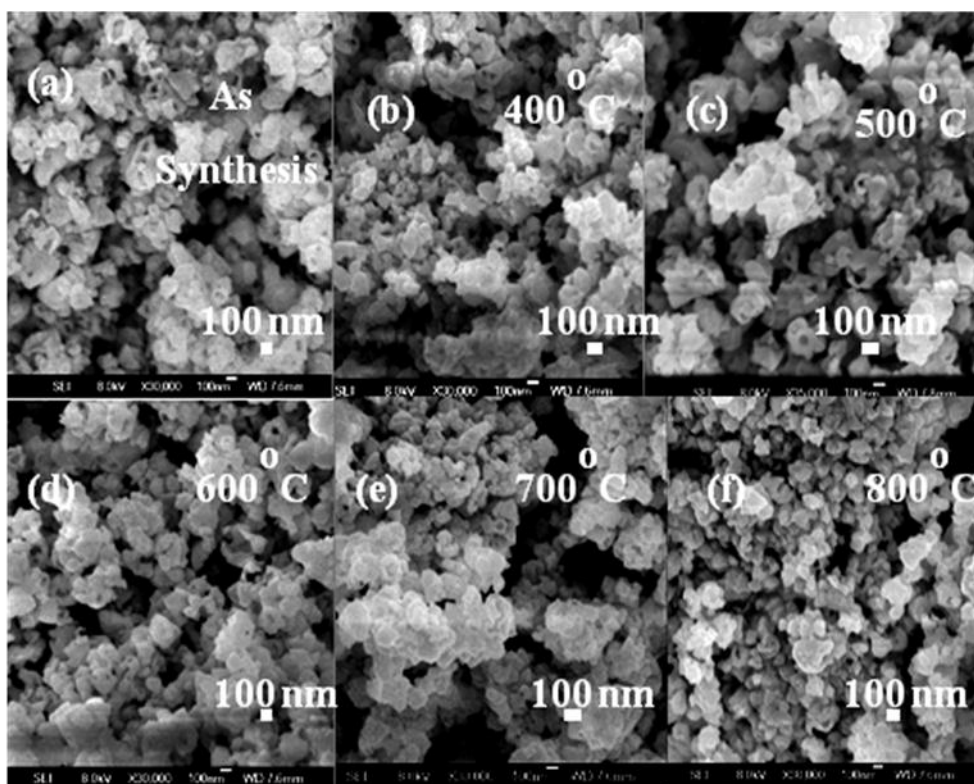


Figure S3 SEM micrographs of solid solution Cd-ZnGeON calcinated at the temperature (a) as synthesised, (b) 400°C, (c) 500°C, (d) 600°C, (e) 700°C and (f) 800°C, where, bar symbol represents 100nm of particle size.

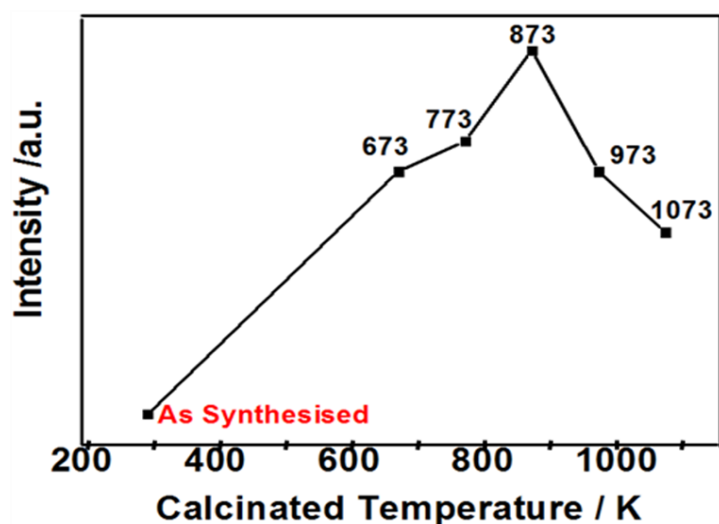


Figure S4 Plot of the intensity of the adsorption peak Vs the calcination temperature.

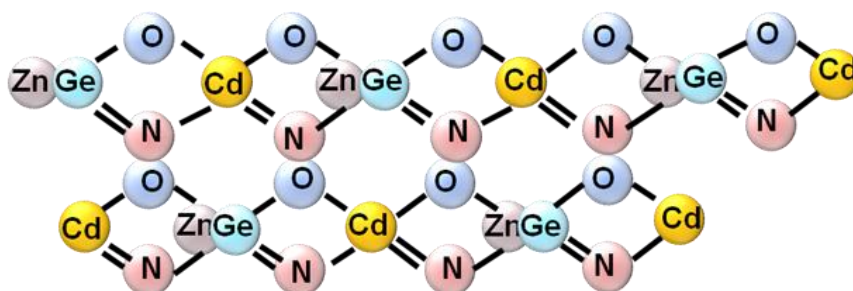


Figure 5S Proposed network of the atomic arrangement in Cd-ZnGeON, as elucidated by XRD, DRS, XPS, and XAS analyses.

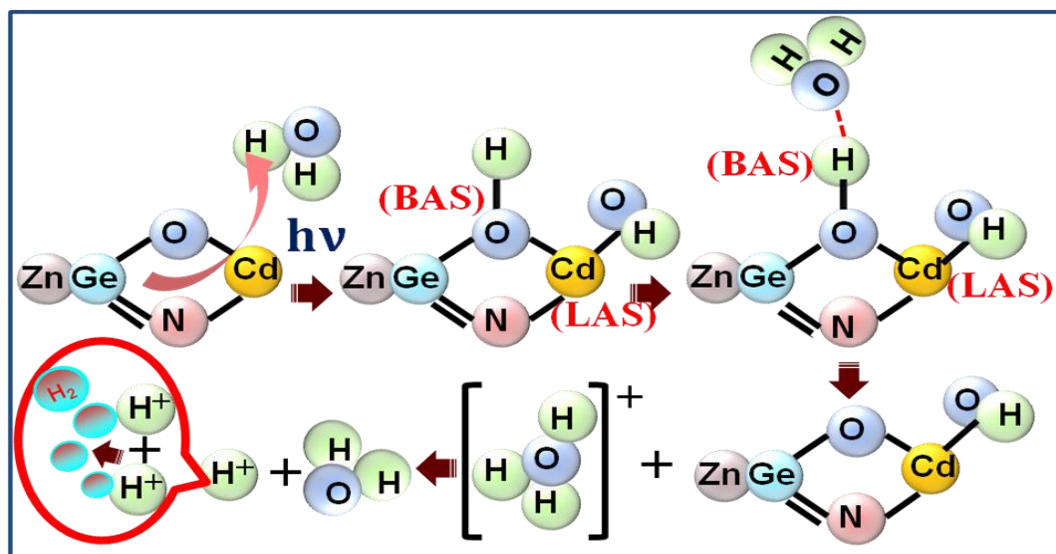


Figure 6S Plausible schematic mechanism of water cleavage for hydrogen generation at active reduction sites, within the lattice cluster network of Cd-ZnGeON.

Tables

Table.1S Elemental analyses, particle size, Zn/Ge ratio, shape and chemical composition, of the Cd-ZnGeON prepared at different temperature from 750-900°C at the same 15 hours-nitridation time.

Temp. (°C)	% N	% O	% Zn	% Ge	% Cd	Particle size (Zn/Ge)	Shape	Chemical Composition
750	49.11	13.14	25.05	11.51	1.19	110-500 nm (2.18)	Small flakes	$\text{Cd}_{0.10} - (\text{Zn}_{2.18}\text{Ge})(\text{N}_{4.26}\text{O}_{1.14})$
800	52.71	9.95	21.56	15.55	0.23	100-250 nm (1.39)	Voluminous popcorn like	$\text{Cd}_{0.01} - (\text{Zn}_{1.39}\text{Ge})(\text{N}_{3.39}\text{O}_{0.64})$
850	59.24	6.56	18.15	16.70	0.10	150-290 nm (1.09)	Flakes	$\text{Cd}_{0.006} - (\text{Zn}_{1.09}\text{Ge})(\text{N}_{3.54}\text{O}_{0.39})$
900	64.43	1.69	15.86	28.49	0.06	100-350 nm and 4-15 μm (0.56)	Smooth cuboids with holes + square rods	$\text{Cd}_{0.002} - (\text{Zn}_{0.56}\text{Ge})(\text{N}_{2.26}\text{O}_{0.06})$

Table.2S Elemental analyses, particle size, Zn/Ge ratio, shape and chemical composition Color coordinates (X, Y, T and dc) cultivated at different excitation wavelength at room temperature, from PLE plots by utilising software CIE13.3 for the solid solution Cd-ZnGeON, prepared at various nitridation temperature.

Nitridation Temp. (°C)	Excitation (nm)	X	Y	T _c (K)	dc(e ⁻⁰²)
800	210	0.2895	0.3368	7692	1.57
850	345	0.5062	0.4603	2508	1.47
900	348	0.3856	0.4418	4260	2.33