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Supporting Information

Structure Analysis and Photocatalytic Properties of Spinel Zinc Gallium Oxonitrides

Venkata Bharat Ram Boppana,[a] Heather Schmidt,[b] Feng Jiao,[a] Douglas J. Doren,[b] and Raul F. Lobo*[a]

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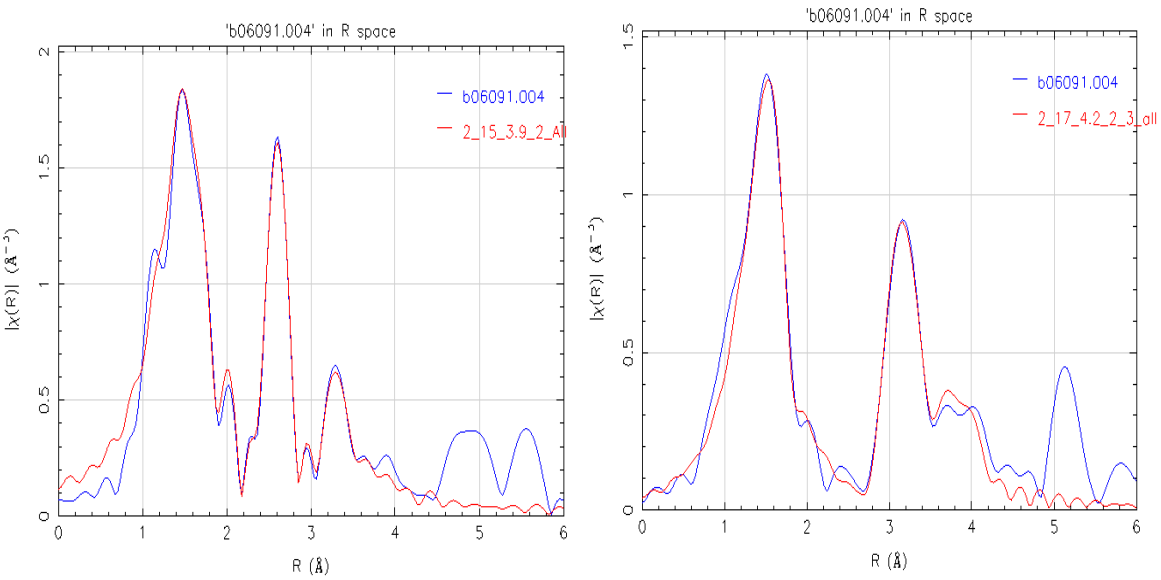

Figure S1. Typical EXAFS refinements of Ga-k edge (A) and Zn k-edge (B), the represented figure is for ZGON 650^{o}C material

The structure file of spinel ZGON used for BS-DOS calculation, $Zn_8Ga_{16}O_{29}N_2Vo_1$

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Zn1:   X=0.75051046 Y=0.73930250 Z=0.75932220
Zn2:   X=0.00183379 Y=0.00323661 Z=0.99898259
Zn3:   X=0.24449948 Y=0.24537033 Z=0.75409846
Zn4:   X=0.49851897 Y=0.50311833 Z=0.99811588
Zn5:   X=0.25296109 Y=0.75291337 Z=0.24853058
Zn6:   X=0.50116009 Y=0.99729325 Z=0.49772798
Zn7:   X=0.74288304 Y=0.25193990 Z=0.26159875
Zn8:   X=0.03696455 Y=0.53536254 Z=0.46001462
Ga1:   X=0.38519498 Y=0.37359000 Z=0.37344300
Ga2:   X=0.37394720 Y=0.62884825 Z=0.62525962
Ga3:   X=0.62607457 Y=0.61804637 Z=0.37717504
Ga4:   X=0.60006977 Y=0.37372588 Z=0.62623791
Ga5:   X=0.87479539 Y=0.87552840 Z=0.37024467
Ga6:   X=0.86806289 Y=0.09882249 Z=0.62710180
Ga7:   X=0.12509687 Y=0.12416300 Z=0.37690095
Ga8:   X=0.12529334 Y=0.87556542 Z=0.62648311
Ga9:   X=0.87139421 Y=0.37660631 Z=0.89991853
Ga10:  X=0.87359375 Y=0.62786696 Z=0.11637378
Ga11:  X=0.11767016 Y=0.62244817 Z=0.87505272
Ga12:  X=0.12902723 Y=0.37442274 Z=0.12581610
Ga13:  X=0.37388626 Y=0.87464306 Z=0.87561685
Ga14:  X=0.37572892 Y=0.12458533 Z=0.12605452
Ga15:  X=0.62227557 Y=0.12346589 Z=0.87694081
Ga16:  X=0.62433434 Y=0.87430044 Z=0.12493783
O 1:   X=0.13688963 Y=0.13469180 Z=0.13887665
O 2:   X=0.60735794 Y=0.61700164 Z=0.62056121
N 1:   X=0.61863627 Y=0.38647762 Z=0.39812566
O 4:   X=0.13592436 Y=0.86714378 Z=0.86316204
O 5:   X=0.86353471 Y=0.86968806 Z=0.13418592
O 6:   X=0.37166700 Y=0.38737520 Z=0.62009978
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O 7: X=0.38056461 Y=0.61640016 Z=0.38899328
O 8: X=0.86547383 Y=0.14610631 Z=0.85577132
O 9: X=0.63317602 Y=0.63798415 Z=0.13613059
O 10: X=0.10426998 Y=0.11589822 Z=0.61598375
O 11: X=0.11311506 Y=0.88603568 Z=0.38783821
O 12: X=0.63551125 Y=0.36140680 Z=0.85663415
O 13: X=0.36650222 Y=0.36220824 Z=0.13418337
O 14: X=0.88461908 Y=0.87483488 Z=0.61270459
O 15: X=0.88620158 Y=0.11387026 Z=0.39342050
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O 20: X=0.63731288 Y=0.86118741 Z=0.36392391
O 21: X=0.36218437 Y=0.86847028 Z=0.63687943
O 22: X=0.88982476 Y=0.37855925 Z=0.12745309
N 2: X=0.88666448 Y=0.60465046 Z=0.88343863
O 24: X=0.36200383 Y=0.13236489 Z=0.36516517
O 25: X=0.13772994 Y=0.63897669 Z=0.63394396
O 26: X=0.61539825 Y=0.11366443 Z=0.11316970
O 27: X=0.61292659 Y=0.88798857 Z=0.88556839
O 28: X=0.14255534 Y=0.36055763 Z=0.36464484
V_O 1: X=0.86300000 Y=0.36300000 Z=0.63700000
O 30: X=0.38656496 Y=0.88761401 Z=0.11338404
O 31: X=0.38586182 Y=0.11321214 Z=0.88684105
O 32: X=0.86662423 Y=0.64097500 Z=0.35720580

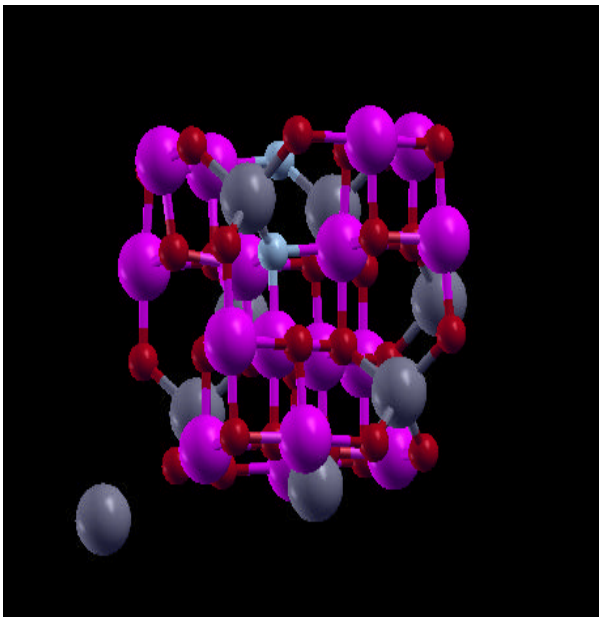

Figure S2. The structure of spinel ZGON ($Zn_8Ga_{16}O_{29}N_2Vo_1$) used for quantum chemical calculations

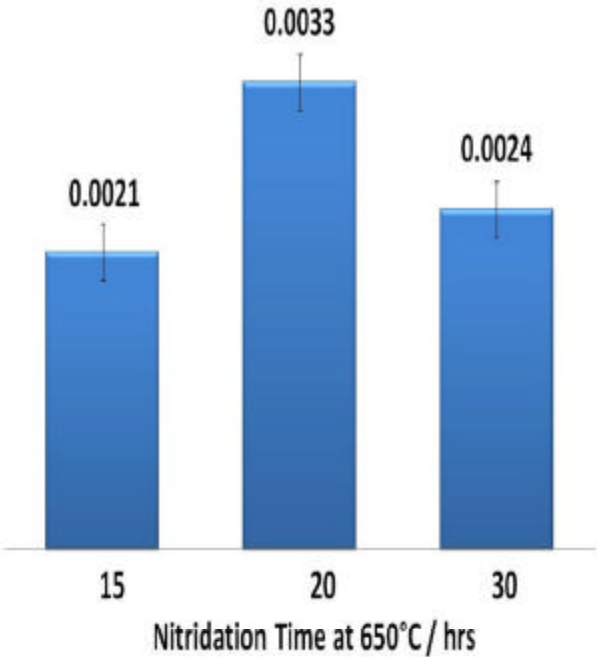

Figure S3. Effective cresol photodegradation rate constants (min^{-1}) for spinel ZGONs synthesized at 650^{o}C at various nitridation times

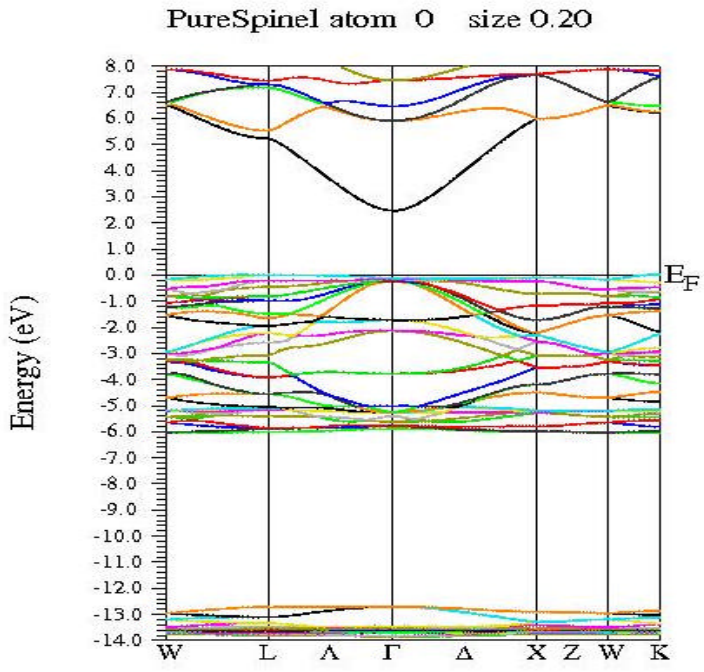

Figure S4. Calculated band structures of spinel zinc gallate ($ZnGa_2O_4$) precursor

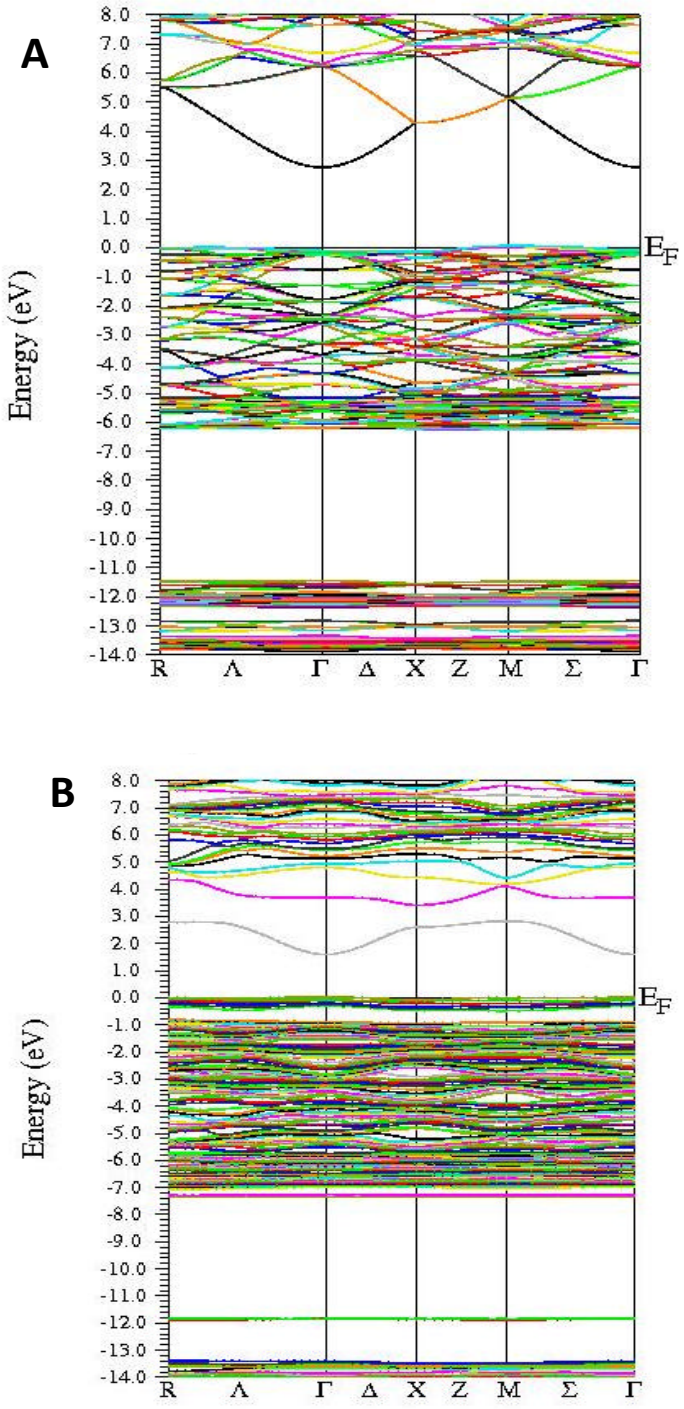

Figure S5. Calculated band structures of spinel zinc gallate precursor ($Zn_8Ga_{16}O_{32}$, A) and spinel ZGON, N 1.32 wt% ($Zn_8Ga_{16}O_{29}N_2[V_O]$, B). The energy scale in each case is set so that the highest occupied state is at zero energy.

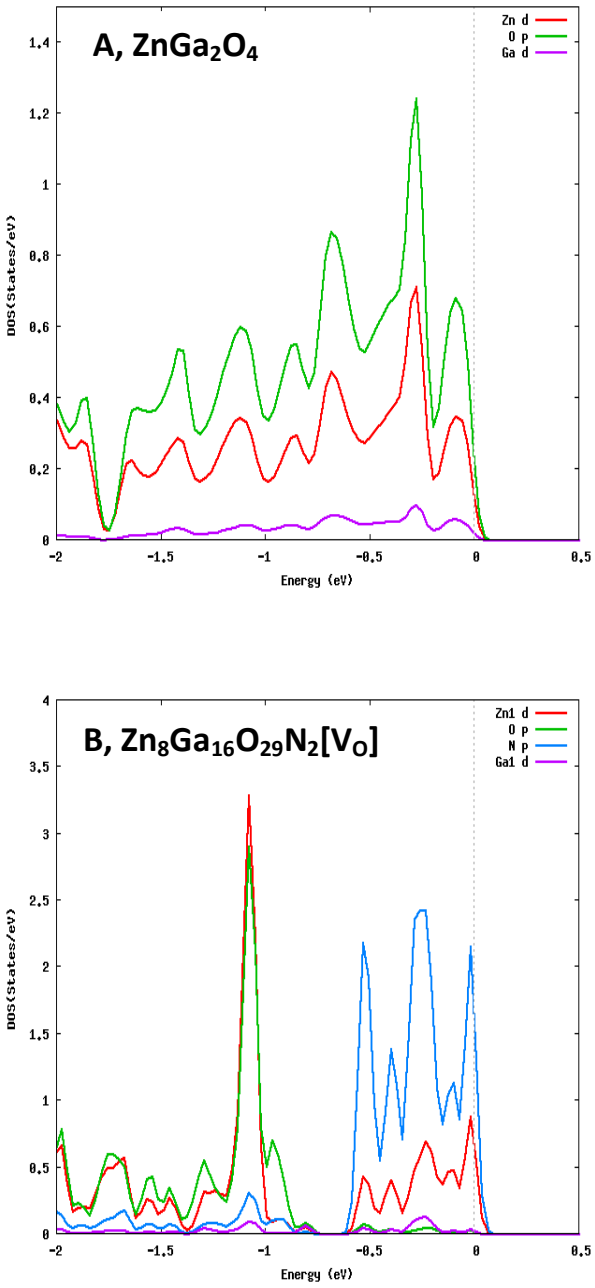

Figure S6. Calculated band structures showing the Zn 3d, O 2p, Ga 3d levels for the spinel zinc gallate precursor (A) and with N 2p orbitals for the spinel ZGON (N content is 1.32 wt%)