Supporting Information for

Sonochemical Synthesis of $ZnCo_2O_4/Ag_3PO_4$ Heterojunction Photocatalysts for the degradation of organic pollutants and pathogens: an experimental and computational study

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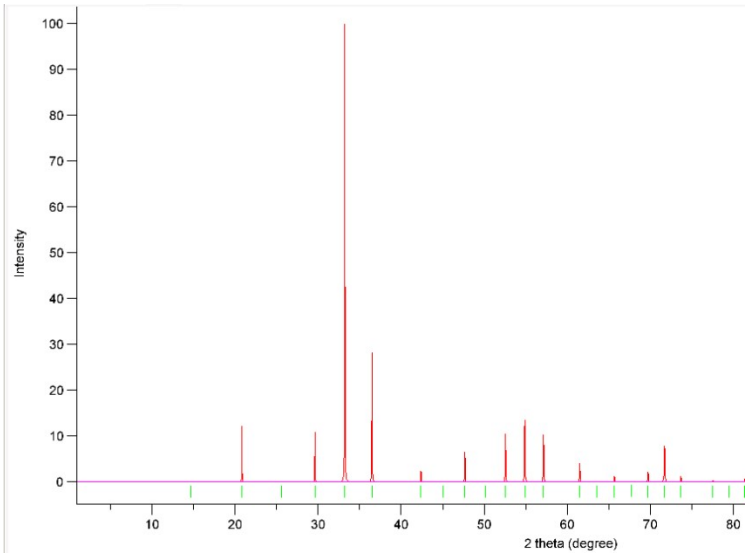
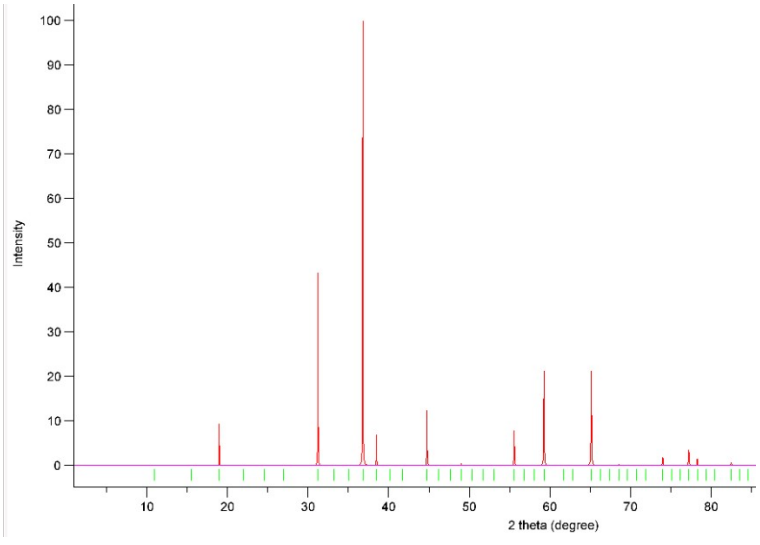
Fig. S0: Simulated powder XRD spectra using the VESTA software [K. Momma and F. Izumi, Commission on Crystallogr. Comput., IUCr Newslett., 7, 106-119 (2006)] of the crystal structures (Cartesian coordinates provided below) used in our *ab initio* calculations. Excellent agreement with our experimental XRD patterns (Top of Fig. 1 of main text) is observed.

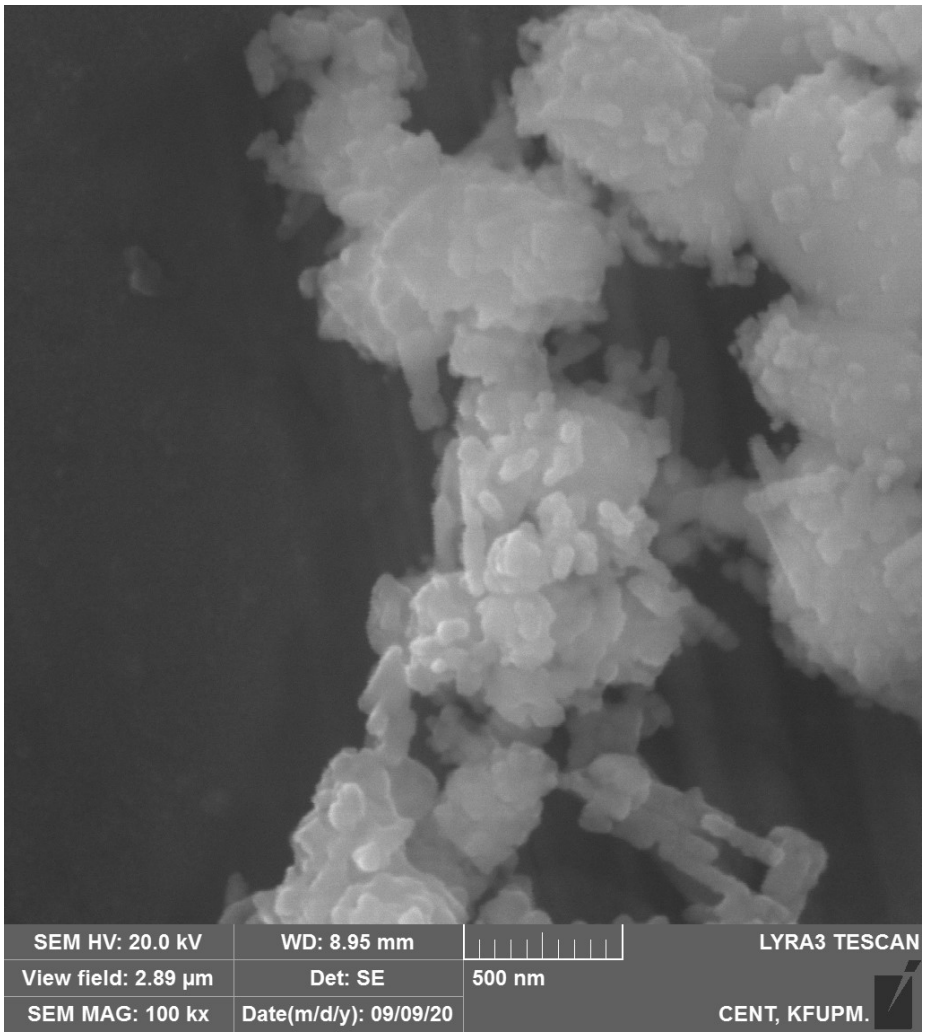


(a) XRD pattern for the experimental geometry of Ag_3PO_4 crystal.



(b) XRD pattern for the relaxed structure of $ZnCo_2O_4$ crystal.

Fig. S1: SEM image of $ZnCo_2O_4/Ag_3PO_4$ nanoparticles



Cartesian coordinates (in Å) for Ag_3PO_4 in xyz format. The computational cell was cubic with a lattice constant of 6.026 Å (experimental value) and contains 6 Ag, 2 P, and 8 O atoms (2 formula units).

16

Ag 0.00000000 3.01300000 1.50650000

Ag 0.00000000 3.01300000 4.51950000

Ag 1.50650000 0.00000000 3.01300000

Ag 4.51950000 0.00000000 3.01300000

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Ag 3.01300000 4.51950000 0.00000000

P 0.00000000 0.00000000 0.00000000

P 3.01300000 3.01300000 3.01300000

O 5.13402545 5.13402545 5.13402545

O 0.89197455 0.89197455 5.13402545

O 0.89197455 5.13402545 0.89197455

O 5.13402545 0.89197455 0.89197455

O 2.12102545 2.12102545 2.12102545

O 3.90497455 3.90497455 2.12102545

O 2.12102545 3.90497455 3.90497455

O 3.90497455 2.12102545 3.90497455

Cartesian coordinates (in Å) for $ZnCo_2O_4$ in xyz format. The computational cell was cubic with a lattice constant of 8.09462 Å (experimental value) and contains 8 Zn, 16 Co, and 32 O atoms (8 formula units).

56

Zn 0.00000000 0.00000000 0.00000000

Zn 0.00000000 4.04731000 4.04731000

Zn 4.04731000 4.04731000 0.00000000

Zn 4.04731000 0.00000000 4.04731000

Zn 6.07096500 2.02365500 6.07096500

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Zn 6.07096500 6.07096500 2.02365500

Co 5.05913750 5.05913750 5.05913750

Co 3.03548250 7.08279250 1.01182750

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Co 5.05913750 3.03548250 3.03548250

Co 5.05913750 7.08279250 7.08279250

Co 1.01182750 1.01182750 5.05913750

O 3.13261794 3.13261794 3.13261794

O 4.96200206 0.91469206 7.17992794

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O 1.10896294 5.15627294 2.93834706

O 6.98565706 6.98565706 6.98565706

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Fig. S2: Calculated band structures. (a) The PBE band structure of Ag_3PO_4 shows an indirect and direct band gap of 0.21 and 0.33 eV, respectively. (b) The PBE band structure of $ZnCo_2O_4$ shows a direct band gap 0.93 eV at the Gamma point. (c) Ag_3PO_4 crystal at the hybrid HSE06 level with a 1/4 fraction of exact exchange shows an underestimated band gap of 1.80 eV.