Supporting Information

Rational design of W-doped Ag_3PO_4 as an efficient antibacterial agent and photocatalyst for organic pollutants degradation

Aline B. Trench,[†] Thales R. Machado,[†*] Amanda F. Gouveia,[‡] Camila C. Foggi,[†] Vinícius Teodoro,[†] Isaac Sánchez-Montes,[†] Mayara M. Teixeira,[†] Letícia G. Trindade,[ǀ] Natalia Jacomaci,[¬] Andre Perrin,[⊥] Christiane Perrin,[⊥] Jose M. Aquino,[†] Juan Andrés,[└] Elson Longo[†*]*

[†] CDMF – Department of Chemistry, Federal University of São Carlos, 13565-905, São Carlos, SP, Brazil.

[‡] Institute of Chemistry, State University of Campinas, 13083-970, Campinas, SP, Brazil.

[ǀ] Department of Chemistry, São Paulo State University, 17033-360, Bauru, SP, Brazil.

[¬] Chemistry Institute, São Paulo State University, 14800-060, Araraquara, SP, Brazil.

[⊥] University of Rennes 1, Campus de Beaulieu, F-35042, Rennes-Cedex, France.

[└] Department of Analytical and Physical Chemistry, University Jaume I, 12071, Castellón, Spain.

Corresponding Author

* E-mail: aline_trench@hotmail.com (A.B. Trench)

*E-mail: tmachado.quimica@gmail.com (T.R. Machado)

*E-mail: elson.liec@gmail.com (E. Longo)

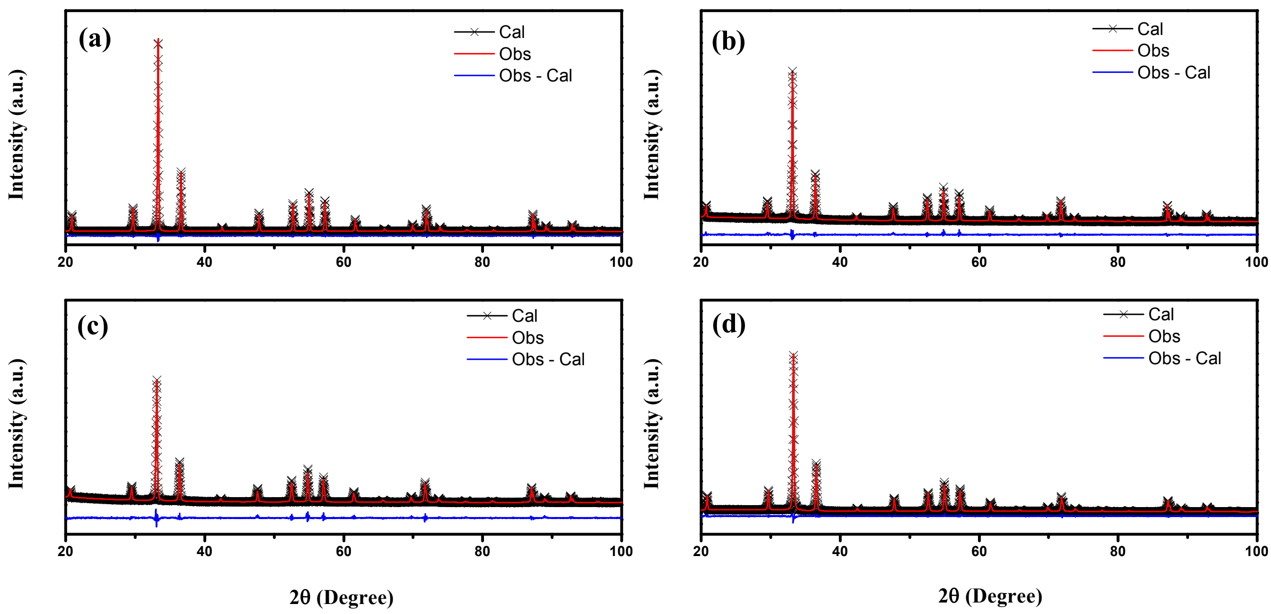

Figure S1. Rietveld refinement plots of pure Ag_3PO_4 (a), Ag_3PO_4: W 0.5% (b), Ag_3PO_4:W 1% (c), and Ag_3PO_4:W 2% (d).

Table S1. Rietveld refinements of pure Ag_3PO_4 and Ag_3PO_4:W powders.

Sample	**Lattice Parameters** a=b=c (Å)	**Cell volume (Å)^3**	**R_{Bragg}**	**χ^2 (%)**	**R_{wp} (%)**	**R_p (%)**
Ag_3PO_4	6.015570(18)	217.6860(20)	0.0605	2.36	8.75	6.43
W 0.5%	6.01740(4)	217.885(5)	0.0636	1.72	6.38	4.82
W 1%	6.01839(7)	217.992(8)	0.0651	1.95	7.45	5.52
W 2%	6.01685(15)	217.825(16)	0.0473	2.38	6.28	4.79

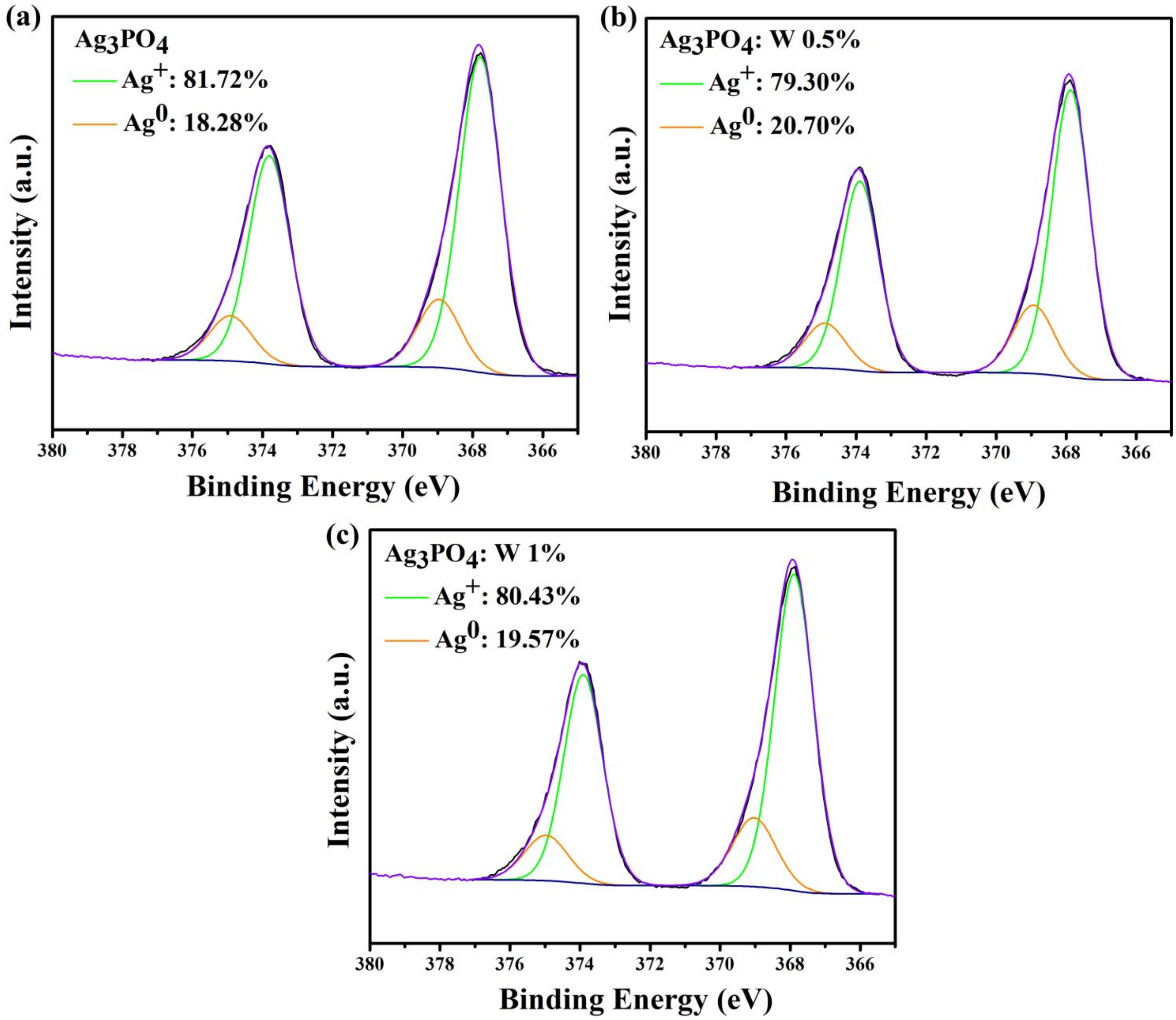

Figure S2. High-resolution XPS spectra of Ag 3d for Ag_3PO_4, Ag_3PO_4: W 0.5%, and Ag_3PO_4: W 1% samples.

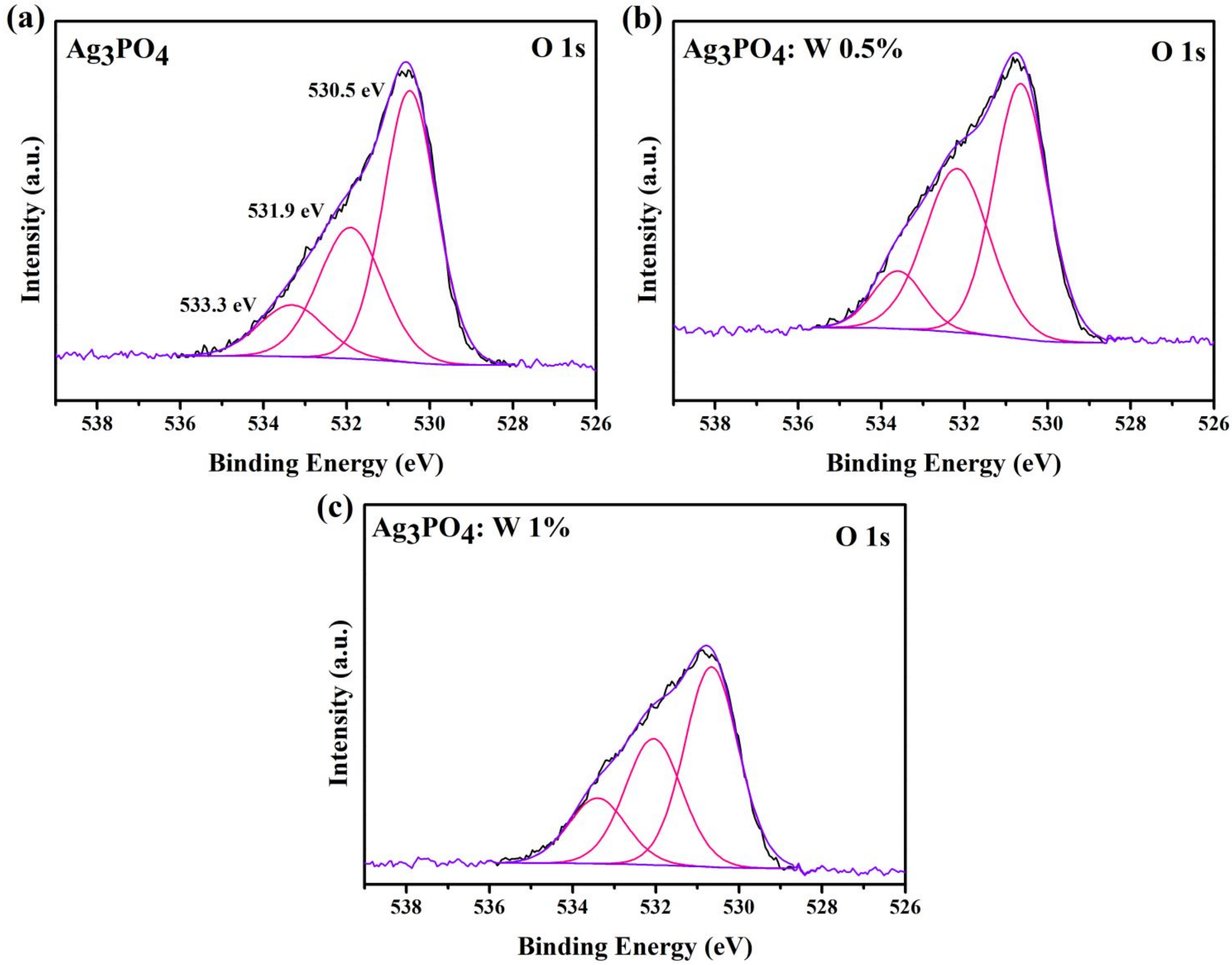

Figure S3. XPS spectrum of O 1s for pure Ag_3PO_4 (a), Ag_3PO_4:W 0.5% (b), and Ag_3PO_4:W1% (c) samples.

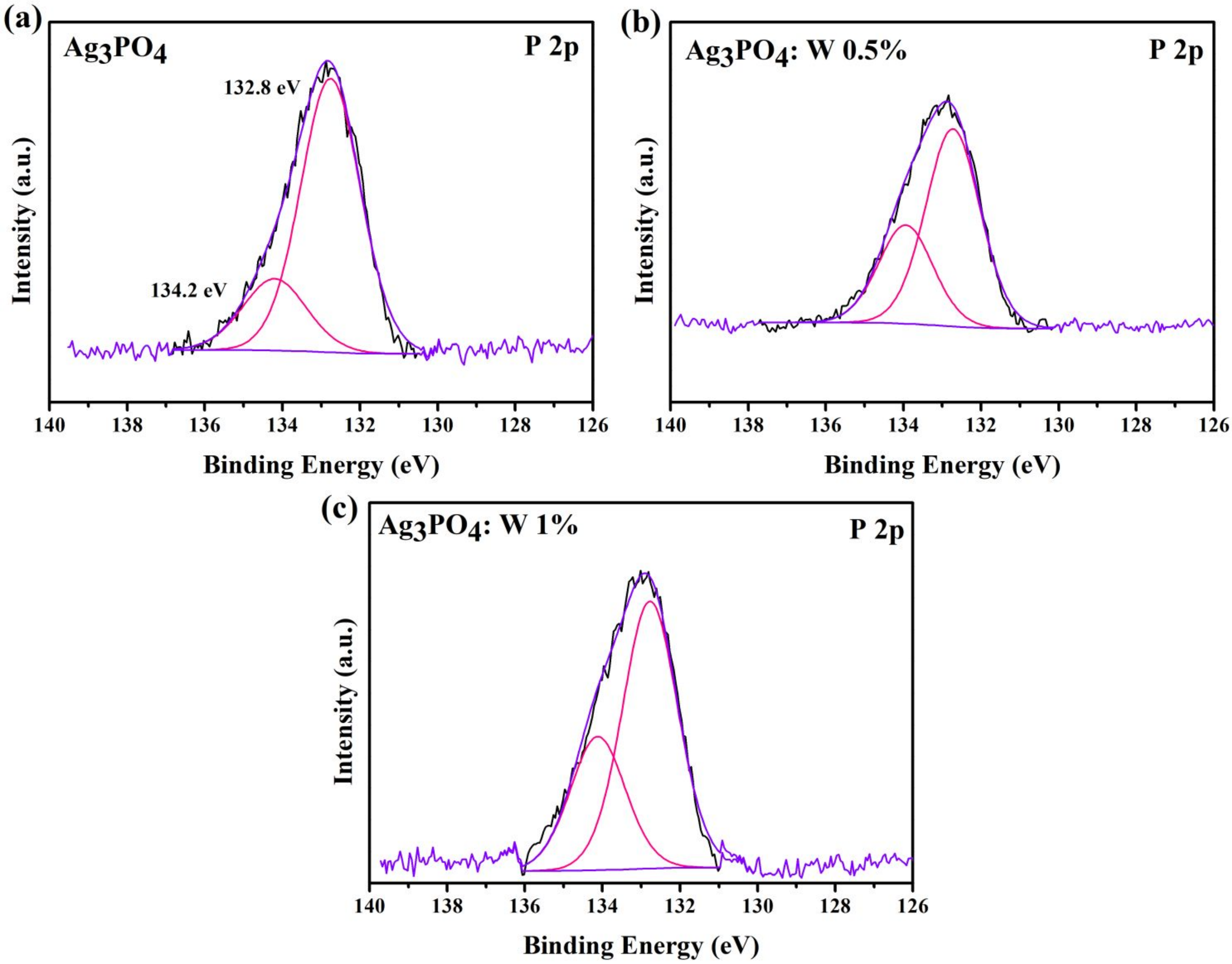

Figure S4. XPS spectrum of P 2p for pure Ag_3PO_4 (a), Ag_3PO_4:W 0.5% (b), and Ag_3PO_4:W 1% (c) samples.

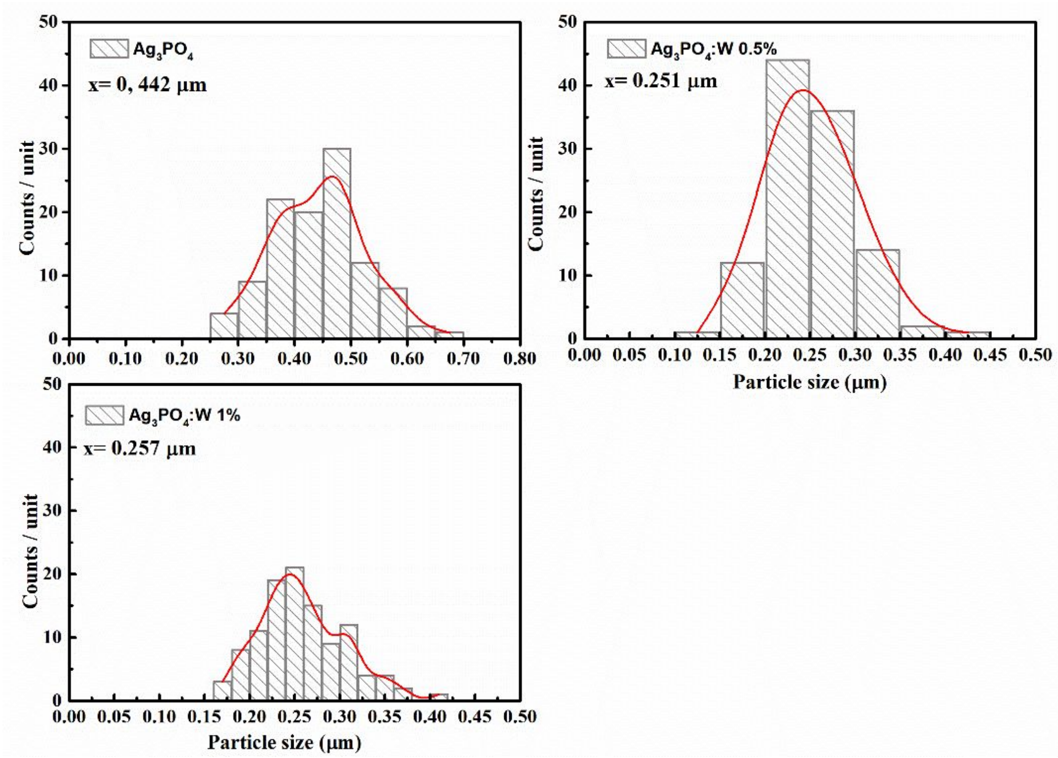

Figure S5. Particle size distribution for Ag_3PO_4, Ag_3PO_4:W 0.5%, and Ag_3PO_4:W 1%.

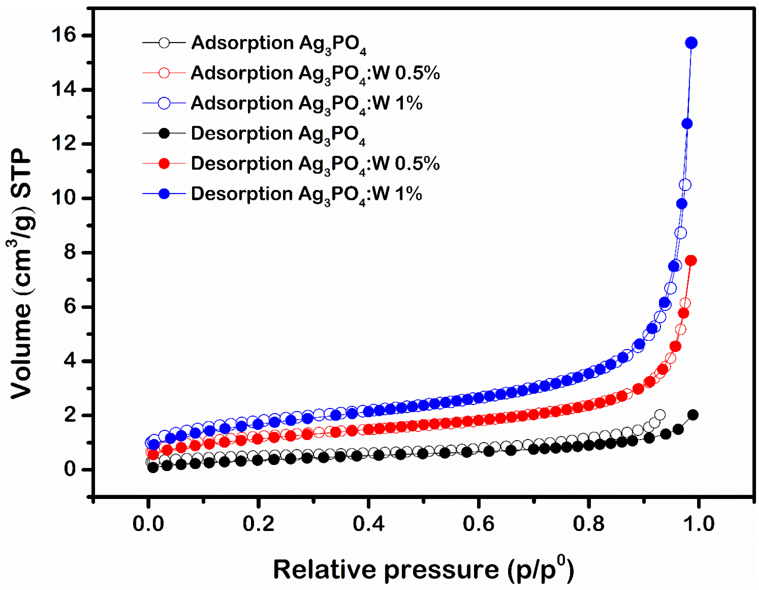

Figure S6. Adsorption-desorption isotherms of Ag_3PO_4, Ag_3PO_4:W 0.5%, and Ag_3PO_4:W 1%.

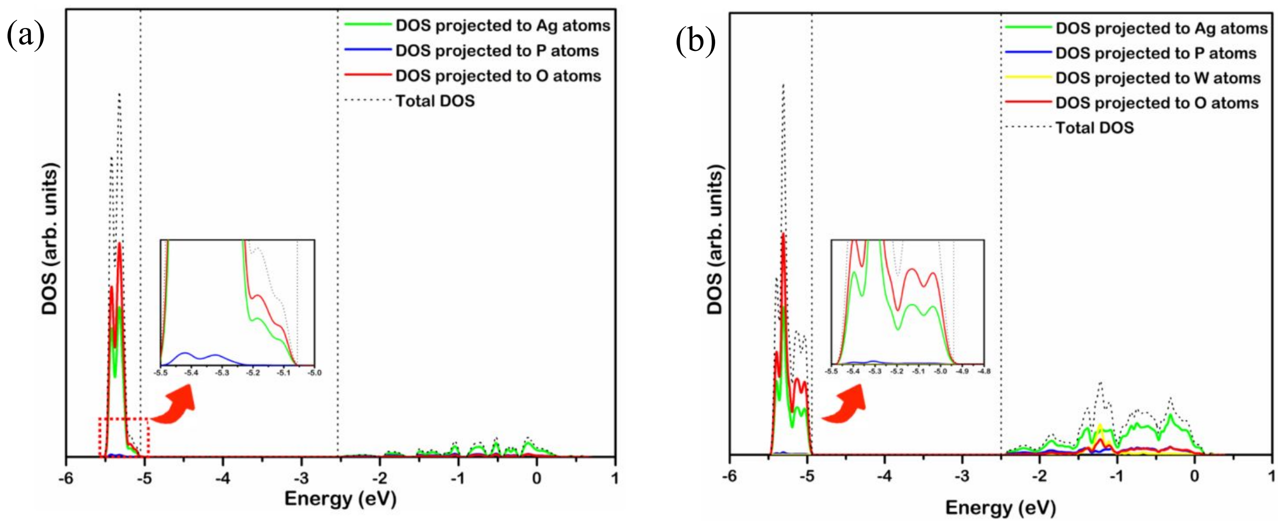

Figure S7. Density of states projected to the Ag, P and O atoms on the (a) Ag_3PO_4 and (b) Ag_3PO_4:W models.