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Supporting Information

2-D Transition Metal Trichalophosphogenide FePS₃ Against Multi-Drug Resistant Microbial Infections

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Supplementary Material



Figure S1. 3-D Structure of mechanically- exfoliated FePS₃ nanosheet (Monolayer)



Figure S2. Additional Characterization of flakes A) STEM image, B) H-R TEM image



Figure S3. XPS analysis of the exfoliatd flakes showing peaks in the (A) iron and (B) sulphur components.



Figure S4. Degradation of FePS₃ nanoflakes. A) STEM image of a degrading FePS₃ nanoflake after 24 hours under ambient conditions. Corresponding EDS images showing B) phosphorus, C) sulphur, and D) oxygen components.



Figure S5: Antimicrobial efficacy of positive controls. (A) Tetracycline was used as a positive control for bacterial strains (MRSA and *P. aeruginosa*) and (B) Fluconazole for *Candida albicans*. The concentrations used for both positive controls are in a range of 0.64-128 μ g/mL. Values are mean \pm SEM. n = 3.



Figure S6. Antimicrobial properties of FePS₃ nanoflakes against a series of fungal population densities. (A) CLSM images of control and treated *C. albicans*. (B) Relative quantification of cell death in fungi. (C) Fungal surface density (number of fungi/ μ m²) of *C. albicans* at different optical densities in both control and FePS₃-treated groups



Figure S7. UV-Vis adsorbance spectra of blank (in red) and FePS₃ treated samples (in green).



Figure S8. Hemolysis assay of FePS₃ nanoflakes against red blood cells. (A) 24 h and (B) 48 h. Cp corresponds to the positive control (C_p), and C_n negative control (treated with 100% ethanol).

Table S1. Table is recreated from Shaw *et al.*, **2021**¹. Comparative antimicrobial activity of commonly investigated nanomaterials. Abbreviations: BP: black phosphorus, NMP: N-methyl-2-pyrrolidone, DMPI: N,N'-dimethylpropyleneurea, PPMS: 4-pyridonemethylstyrene, NPs: nano-particles, NB: Not bactericidal, N/A: Not applicable, NR: Not reported. Material 1 highlighted in blue is that of this study.

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				Bacteria	Fungi	Cytotoxicity	Bactericidal Activity	Bacterial Treatmen t Times	Fungicidal Activity	Bactericidal Treatment time
Mechanically Exfoliated FePS ₃	Size: 2-4µm Thickness: 65nm	816.7 ng/cm ²	No	MRSA, P.aeruginosa	C.albicans	No	99.99% (MRSA) and 99.9% (<i>P.aeruginosa</i>)	4 hours	50% (C.albicans)	4 hours
Mechanically Exfoliated BP	Size: 500 nm - 5 μm Thickness: 15 – 90 nm	~900 ng/cm ²	No	E. coli, P. aeruginosa, MRSA, S. typhimurium, and B. cereus	<i>C. albicans</i> , <i>C. auris</i> and sensitive, fluconazole- resistant, and Amphotericin B-resistant <i>C.</i> <i>neoformans</i> .	No	96.3% (E.coli) and 96.2% (P. aeruginosa)	2 hours	99.92% (C. albicans) and 99.3% (C. neoformans {F ^R })	2 hours
NMP - BP with Ti-SA ₄ ²	Size: 220 nm Thickness: 5 nm	50 μg/mL	No	E. coli & S. aureus	No	NR	99.2% (E. coli), 94.6 % (S. aureus).	3 hr	NR	NR
DMPU - BP ³	Size: 0.1 - 4 μm. Thickness: 2 - 15.4 nm	160 μg/mL	Yes, NIR irradiation at 808 nm.	E. coli & S. aureus	No	NR	99.2%	3 - 10 min	NR	NR

Ag and BP nanosheets ⁴	AgNPs: 30 nm BP: 220 nm Thickness: 4 nm	25 - 40 μg/mL	Yes; NIR irradiation at 808 nm.	MRSA	No	No	93%.	5 min	NR	NR
DCM - BP with PPMS ⁵	Size: microns Thickness: 4.2 - 4.5 nm	100 µg/ml	Yes; irradiation at 660 nm	E. coli & S. aureus	No	No	99.3% & 99.2% (E. coli), 76.5% & 69.5% (S.aureus).	10 min	NR	NR
Millipore water - BP	Size: 215.8 nm Thickness: 1.6 nm	50- 100 μg/mL.	No	E. coli & B. subtilis	No	NR	91.65% & 99.69%	6 - 12 hr	NR	NR
Au-BP Nanosheets ⁶	Size: >100 nm Thickness: 2 nm	<10 µg/mL	No	E. coli	No	NR	94.7%	8 hr	NR	NR
BP-TiO ₂ ⁷	NR	25 μg/mL	Yes; UV- vis	E. coli & S. aureus	No	NR	NR	70 min	NR	NR
MoS ₂ Composites ^{8,} 9	Size: NR Thickness: 2.2 nm	≤1 mg/mL	Yes, NIR ⁸	E. coli & S. aureus	No	Concentration & system dependent ^{10, 11}	100%	≤6 hr	NR	NR
Ag NPs ¹²	Size: 4 - 24 nm	50 μg/mL	No	E. coli	Yes ¹³⁻¹⁶	Yes; shape & concentration dependent ¹⁷	100%	24 hr	Varying degrees. ^{15, 18}	NR
Au NPs ¹⁹	Size: 10 - 200 nm	Widely Variant	No	Controversial ¹⁹	Yes; ^{20, 21} controversial	Dose & size dependent ²⁴	NB	N/A	MIC: 4 - 48 μg/mL	NR
ZnO NPs ^{25, 26}	Size: 50 - 250 nm	0.25 g/L	Yes, UV- vis ^{25, 26}	E. coli & S. aureus	Numerous Species ²⁷⁻²⁹	Yes ³⁰⁻³²	Conditional, but >99%	2 hr	Yes ^{28, 29, 33}	NR

Graphene oxide (pure & reduced) ³⁴	Size: ~0.31 μm Size: ~2.75 μm	80 μg/mL	No	E. coli	Yes; ³⁵ enhanced with NIR ³⁶	Morphology, chemistry, sys dependent ^{37, 38}	Pure: 90% Reduced: 80%	2 hr	$\frac{IC_{50}:50-}{100}\\ \mu g/m L^{35}$	NR
Graphene oxide ³⁹	Size: 5 - 20 µm Thickness: 1.2 nm	200 μg/mL	No	None for pure graphene oxide	NR	NR	0%	N/A	NR	NR
TiO ₂ NPs ⁴⁰	Size: 79 nm	1200 μM	UV- visible Light	E. coli	Yes ⁴¹ , surface additive ^{42, 43}	Yes, concentration- & time- dependent manner. ⁴⁴	75% reduction	N/A	Yes ^{41, 45}	NR
Cu-TiO ₂ NPs ⁴⁶	Size: 15-50 nm	1 mg/mL	UV-vis	E. coli	NR	NR	100% reduction	N/A	NR	NR
Au nanostar ⁴⁷	Size: 50 – 100 nm	Monolayer of nanostar on glass	NIR laser	S. aureus	NR	NR	99%	30 min	NR	NR
Au nanocross ⁴⁸	Size: ~100 nm	0.2 mg/mL	NIR laser	P. aeruginosa	NR	NR	99%	5 min	NR	NR

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