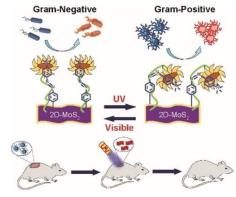
#### **Summary of 10 selected paper:**

1. Photo-Controlled Gating of Selective Bacterial MembraneInteraction and Enhanced Antibacterial Activity for Wound Healing. (Angew. Chem. Int. Ed. 2024, 136, e202314804.)

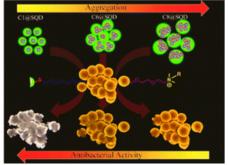
We present a photoswitchable bio-interface through ligand functionalization on 2D-MoS<sub>2</sub>, achieving differential-interactions-based Gram-selective antibacterial activity that enables effective wound healing applications. We have shown the detail mechanisms for the selective antibacterial activity. We found strain-specific and high bactericidal activity (minimal bactericidal concentration,  $0.65~\mu g/ml$ )



with low cytotoxicity, which we extended to wound healing applications. This methodology provides a single platform for efficiently switching between conformers to reversibly control the strain-selective bactericidal activity regulated by light.

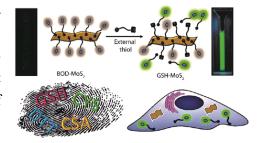
### 2. Post-functionalization of sulfur quantum dots and their aggregation-dependent antibacterial activity. (Nanoscale 2023, 15, 18624-18638.)

We explored the surface functionalized nanometallic nanomaterials with very high antibacterial activity (10–25 ng ml<sup>-1</sup>) which is 10<sup>5</sup> times higher compared to that of nonfunctionalized same system. This development is highly important, as this system can be used for several biomedical applications. More importantly, a rare phenomenon of the reverse trend of antibacterial activity through surface modification was observed. In general, with increasing surface hydrophobicity of various nanomaterials, the antibacterial activity increases. However, for the first time we reported



the surface hydrophobicity increased, the nano antibiotics tended to exhibit a propensity for aggregation, which consequently decreased their antibacterial efficacy. This identical pattern was also evident in *in vivo* assessments.

**3. Ligand Exchange on MoS<sub>2</sub> Nanosheets: Applications in Array-Based Sensing and Drug Delivery.** (ACS Nano **2022**, 17, 1000-1011.) In this study, we have observed the ligand-exchange phenomenon on 2D-MoS2 in the presence of different thiolated ligands. Further, this concept was applied to a cancerous cell line for in vitro delivery and detection of various biologically related thiols in biofluids.



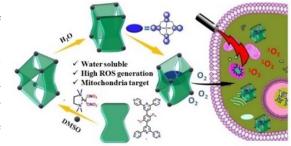
#### 4. 2D-MoS<sub>2</sub>-supported copper peroxide nanodots with enhanced nanozyme activity: application in antibacterial activity. (*Nanoscale* 2023, 15, 19801-19814.)

In this study, we prepared a MoS2-based nanocomposite with copper peroxide nanodots (MoS2@CP) to achieve pH-dependent light-induced (NIR) nanozyme-based antibacterial action. It has shown superior peroxidase and antibacterial activity at low pH. This work highlighted the combinatorial approach for eradicating bacterial infections using enzyme-based antibacterial agents.



# 5. Solvent Induced Conversion of a Self-Assembled Gyrobifastigium to a Barrel and Encapsulation of Zinc - Phthalocyanine within the Barrel for Enhanced Photodynamic Therapy. (Angew. Chem. Int. Ed. 2023, 135, e202218226.)

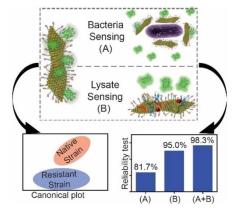
In this work, we have demonstrated the use of molecular cage (MC) for application of aqueous insoluble therapeutic molecules. We have encapsulated zinc-phthalocyanine (ZnPc) in a self-assembly of a tetradentate donor (L) with PdII acceptor and observed an excellent photosensitizer for photodynamic therapy (PDT). Higher cellular uptake and anticancer activity of the ZnPc⊂MC compared to free ZnPc on HeLa cells indicate that



encapsulation of ZnPc in an aqueous host is a potential strategy for enhancement of its PDT activity in water.

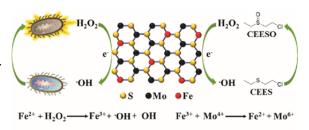
## **6.** Rapid Discrimination of Bacterial Drug Resistivity by Array-Based Cross-Validation Using 2D MoS<sub>2</sub>. (*Chem. Eur. J.* 2022, 28, e202201386.)

A sensor array comprising cationic 2D MoS<sub>2</sub> and GFP has been used to discriminate bacterial analytes. By using this optimized sensor array, bacteria and lysates belonging to different types and with different amounts of drug resistivity were successfully classified. Cross validation of blind samples through combined analysis of bacterial cell and lysates provided improved detection accuracy.



### 7. Fe-Doped MoS<sub>2</sub> nanozyme for antibacterial activity and detoxification of mustard gas simulant. (ACS Appl. Mater. Interfaces 2022, 14, 42940-42949.)

In this study, we have demonstrated the preparation of Fedoped MoS<sub>2</sub> (Fe@MoS<sub>2</sub>) nanomaterials with enhanced peroxidase-like activity of MoS<sub>2</sub> in a co-catalytic pathway. The efficient decomposition of H2O<sub>2</sub> in the presence of Fe@MoS<sub>2</sub> has been employed toward the antibacterial activity and detoxification of mustard gas simulant. This

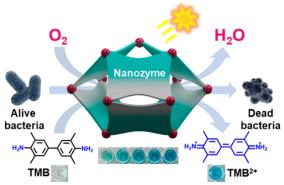


 $Peroxidase-like\ Co-Catalytic\ Activity\ of\ Fe@MoS_2$ 

work demonstrates the development of a hybrid nanozyme and its environmental remediation from harmful chemicals to microbes.

### 8. Self-Assembled Pd<sub>12</sub> Coordination Cage as Photoregulated Oxidase-Like Nanozyme. (*J. Am. Chem. Soc.* 2020, 142, 18981-18989.)

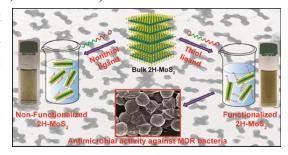
We reported a water-soluble  $Pd_{12}$  nanocage with excellent oxidase-like activity upon irradiation with white light. The benzothiadiazole unit in the structure helped in the photogeneration of reactive oxygen species (ROS) in water. The enzymatic activity of nanocage is photoregulated which offers other obvious advantages, such as external control of enzymatic



activity and noninvasiveness. The oxidase-like activity and exogenous ROS generation have been exploited in photocatalytic antibacterial activity against methicillin-resistant *Staphylococcus aureus* (MRSA) bacterial strain.

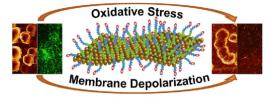
### 9. Simultaneous Exfoliation and Functionalization of 2H-MoS<sub>2</sub> by Thiolated Surfactants: Applications in Enhanced Antibacterial Activity. (J. Am. Chem. Soc. 2018, 140, 12634-12644.)

We reported a new method for the exfoliation and direct functionalization of 2H-MoS<sub>2</sub> using surfactant molecules with thiol functionality. We found that the exfoliated MoS<sub>2</sub> using thiolated ligands are functionalized with desired functionality and the processing scheme can be extended to other TMDs. Functionalized 2H-MoS<sub>2</sub> exhibits highly enhanced antibacterial efficiency compared to similarly functionalized metallic 1T-MoS<sub>2</sub> against pathogenic bacteria.



### **10.** High Antibacterial Activity of Functionalized Chemically Exfoliated MoS<sub>2</sub>. (ACS Appl. Mater. Interfaces **2016**, 8, 31567-31573.)

This paper reports a proof-of-principle study to evaluate the potential of functionalized two-dimensional chemically exfoliated MoS2 (ce-MoS2) toward inhibitory and bactericidal property against two representative ESKAPE pathogenic strain—a Grampositive Staphylococcus aureus (MRSA) and a Gram-negative



Pseudomonas aeruginosa. A comparison with widely used small molecules and other nanomaterial-based therapeutics conclusively establishes a better efficacy of 2D ce-MoS2 as a new class of antibiotics.