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**Oral Abstract**

**Ni/Ni<sub>3</sub>S<sub>2</sub> Nanoparticles Embedded in Porous S-doped Carbon Nanosheet Arrays for Enhanced Hydrogen Evolution**

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**Abstract**

Three-dimensional (3D) carbon-based catalysts grown on a substrate exhibit superior electrocatalytic activities towards hydrogen evolution reaction (HER).<sup>1,2</sup> We herein describe a novel method for *in situ* fabrication of hybrid Ni/Ni<sub>3</sub>S<sub>2</sub> nanoparticles embedded in S-doped carbon nanosheet arrays (Ni/Ni<sub>3</sub>S<sub>2</sub>/SC NSAs) on carbon cloth. With the morphological merits of large surface area and high conductivity, Ni/Ni<sub>3</sub>S<sub>2</sub>/SC NSAs are demonstrated as an efficient and durable HER catalyst that requires merely 90 mV at a current density of 10 mA cm<sup>-2</sup> with a small Tafel slope of 81 mV dec<sup>-1</sup>. This excellent performance is ascribed to the formation of Ni<sup>δ+</sup> and S<sup>δ-</sup> species that promote the cleavage of H-OH bonds. First-principles calculations further reveal that the Ni surface near the Ni/Ni<sub>3</sub>S<sub>2</sub> interface has a larger water adsorption energy ( $E_{ad}$ ) and lower activation energy for water dissociation ( $E_a$ ) than pure Ni and Ni<sub>3</sub>S<sub>2</sub>, which contribute to enhance HER performance. This work offers valuable insights into the designing of interface between transition metal-based catalysts and heteroatom-doped carbon materials.

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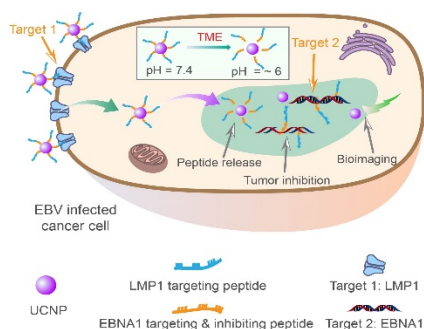
**Dual-targeting peptide-guided approach for precision delivery and cancer monitoring using a safe upconversion nanoplatform**

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**Abstract**

Using EBV-induced and HeLa cancer cells as a comparative study model, a novel and safe dual-EBV-oncoproteins-targeting pH-responsive peptide engineering, coating and guiding approach to achieve precision targeting and treatment strategy against EBV-associated cancers is demonstrated. Individual functional peptide sequences that specifically bind to two overexpressed EBV-specific oncoproteins, EBNA1 (a latent cellular protein) and LMP1 (a transmembrane protein), are engineered in three different ways and incorporated with a pH-sensitive tumor microenvironment (TME)-cleavable linker on to the upconversion nanoparticles (UCNP)  $\text{NaGdF}_4:\text{Yb}^{3+}, \text{Er}^{3+}@\text{NaGdF}_4$  (UCNP-P<sub>n</sub>, n = 5, 6 and 7). A synergistic combination of the transmembrane LMP1 targeting ability and the pH responsiveness of UCNP-P<sub>n</sub> was found to give specific cancer differentiation with higher cellular uptake and accumulation in EBV-infected cells. This lowered the effective dose, reducing potential side effects and health risks from treatment. The approach also gives responsive UC signal enhancement upon targeted dual-protein binding and showed effective EBV cancer inhibition in vitro and in vivo. This is the first example of simultaneous imaging and inhibition of two EBV latent proteins, and serves as a blueprint for a next-generation peptide-guided precision delivery nanosystem for the safe monitoring and treatment against a specific cancer.



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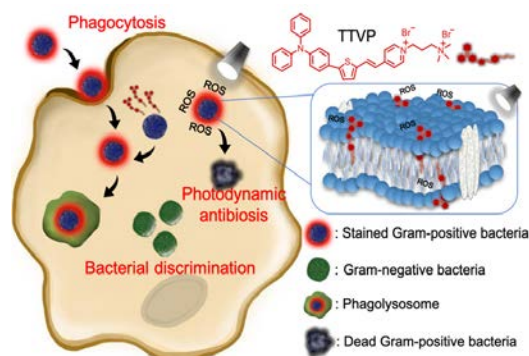
**Highly efficient phototheranostics of macrophage-engulfed Gram-positive bacteria  
using a NIR luminogen with aggregation-induced emission characteristics**

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**Abstract**

Although phagocytosis serves as the front line to attack invading pathogens, its low bacterial encounter and killing rates leads to an ineffective bactericidal output. In view of this, developing multifunctional theranostic probe to effectively discriminate and ablate intracellular bacteria is highly desirable. However, the shielding effect of the host macrophages put the detection and elimination of macrophage-engulfed bacteria into a challenging task. Herein, we utilize a luminogen with aggregation-induced emission (AIE) characteristics, namely TTVP, as a simple and effective probe for simultaneous tracing and photodynamic killing of intracellular Gram-positive bacteria.<sup>1</sup> With the help of the AIE property, excellent water solubility, near-infrared (NIR) emission and strong reactive oxygen species (ROS) generating ability, TTVP performed ideally to be a targeting agent to intracellular Gram-positive bacteria with high signal contrast, as well as to be a photosensitizer to effectively ablate intracellular bacteria without attacking host macrophages. This work thus provides insights for the next generation antibiosis theranostic application for potential clinical trials.



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**A Versatile molecular carrier utilizing polymeric metal-organic cage micelles:  
biomedical applications**

HKU - Ho Yan Lum Yannis

A bispyridine ligand and a divalent metal ion were employed to construct a metal-organic cage with a molecular formula  $M_{12}L_{24}$  [ $M = Pd^{2+}$  or  $Pt^{2+}$ ]. The cages were endohedrally decorated with functional groups that assists proteins encapsulation and direct covalent linkage of small molecules to perform biomedical tasks. We have 3 types of target encapsulation: *Streptavidin* protein, *Fluorescence Activation Shift Tag (FAST)* protein and small anticancer molecules: *camptothecin (CPT)*. The corona of the cages were fabricated with poly(methoxy-2-ethoxy-2-ethoxyethyl-*N*-glycine) for *FAST* cages, poly(ethylene glycol) for *Streptavidin* cages, and poly(ethylene glycol)-*block*-poly(caprolactone) for *CPT* cages, to enlarge particle size with solubility improvement in water. The polymeric metal-organic cages (polyMOCs) appeared as spherical micelles after aqueous transfer, 13-20 nm in diameter, under Uranyl acetate stained TEM. The successful encapsulation of *Streptavidin* protein to be revealed by CryoEM technique. The encapsulation and the performance of *FAST* cages are yet to be characterized. The *CPT* cages are incorporated with *doxorubicin (DOX)* during aqueous transfer such that a multi-compartment encapsulation is achieved for multi-drug delivery. We predict a decreased  $IC_{50}$  value compared to our previous solely *DOX* system and lengthened life expectancy for the test objects.

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**Polymer Coating on Magnesium Substrates for Orthopaedic Applications**

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Magnesium (Mg) and its alloys show excellent potential as orthopedic implantable materials due to their unique properties, such as high biocompatibility, good biodegradability and favorable mechanical strength. In addition, their *in vivo* degraded Mg ions ( $Mg^{2+}$ ) are known to be capable of promoting the growth of new bone. However, the swift corrosion process during implantation has greatly hindered its clinical applications. An effective method to counter the high rate of corrosion is to coat Mg substrates on surfaces with a thin layer of biodegradable polymer. To achieve long-term corrosion resistance, a biodegradable poly (L-lactic acid) (PLLA) coating on pure Mg substrates (99.99 wt.%) with tunable surface morphologies was fabricated through dip-coating in combination with mixed non-solvent induced phase separation (Dip-coating-mNIPS) method. Our findings illustrated that through the Dip-coating-mNIPS method, the structure of PLLA membrane on Mg substrates could easily be controlled to regulate the corrosion behaviors and improve the biocompatibility. While such a coating reduces the long-term corrosion rate, it prevents the short-term release of bone simulating  $Mg^{2+}$  after orthopedic operations. To balance these contradicting short- and long-term characteristics, we further designed a polymer-inorganic composite coating on pure Mg substrates that enables Mg-based implants to achieve controllable release of  $Mg^{2+}$  and high corrosion resistance simultaneously. The coatings were fabricated by adding an appropriate amount of inorganic magnesium sulfate heptahydrate ( $MgSO_4 \cdot 7H_2O$ ) salt particles into a biodegradable poly (L-lactic acid) (PLLA) polymer matrix, such that they can percolate inside to form an interconnected morphology during the phase separation between Mg salt and PLLA polymers as solvent evaporates during the drying process, resulting in the formation of an organic-inorganic composite coating. The experimental results demonstrated that the incorporation of a suitable amount of Mg salt particles could

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further promote the cytocompatibility as compared to the pristine PLLA coating, suggesting that the composite coating can be potentially applied for future clinical uses.



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**Highly efficient all-inorganic perovskite solar cells with suppressed  
non-radiative recombination by a Lewis base**

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All-inorganic perovskite solar cells (PVSCs) have drawn increasing attention because of their outstanding thermal stability.[1] However, their performance is still inferior than the typical organic-inorganic counterparts, especially for the devices with p-i-n configuration, mainly due to severe energy loss in trap sites of perovskite film and mismatched energy level among each layers.[2]

This study has successfully employed a simple molecular passivation strategy to reduce energy loss by reducing the density of surface defects in perovskite film with  $\pi$ -conjugated 6TIC-4F, which can be dissolved in antisolvent to passivate uncoordinated defects on surface/grain boundaries. Theoretical calculations and experimental characterizations revealed that the numerous nitrogen (N) atoms possessing lone pair electrons on 6TIC-4F could passivate the surface defects of perovskite film via direct coordination with the lead ion ( $\text{Pb}^{2+}$ ) through the formation of Lewis adducts, thereby suppressing the non-radiative recombination in the derived PVSCs. Meanwhile, the

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employed 6TIC-4F tends to trigger the nucleation of perovskite precursor, leading to the formation of larger grain size and denser film. Furthermore, 6TIC-4F possesses a LUMO level of about  $-4.14$  eV, which sits between the CBM of perovskite ( $-3.49$  eV) and ZnO ( $-4.25$  eV). [3] It enables a better energy alignment across the perovskite/ETL interface to provide improved electron extraction efficiency. Consequently, the as-optimized device with the structure of ITO/ NiO<sub>x</sub>/perovskite/ZnO/C60/Ag can deliver a remarkable PCE of 16.1% and a certificated value of 15.6% with much enhanced open-circuit voltage from 1.10 V to 1.16 V, representing the best inverted all-inorganic PVSCs reported thus far.

This work provides an insight in the design of functional interlayers for improving efficiencies and stability of all-inorganic PVSCs.

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**Room Temperature Synthesis of Stable, Printable Cs<sub>3</sub>Cu<sub>2</sub>X<sub>5</sub> (X=I, Br/I, Br, Br/ Cl, Cl) Colloidal Nanocrystals with Near Unity Quantum Yield Green Emitters (X=Cl)**

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**Abstract**

Lead halide perovskite nanocrystals (NCs) have shown remarkable properties for emission applications but their toxicity and instability are a hindrance to many commercial uses. Herein, we report the synthesis of lead-free all-inorganic Cs<sub>3</sub>Cu<sub>2</sub>X<sub>5</sub> (X=I, Br/I, Br, Br/ Cl, Cl) colloidal nanocrystals as members of the metal-metal halide family of materials. These nanocrystals have uniform sizes less than 10 nm in diameter and show excellent optical properties including composition tunable emission spectra over the spectral region of 440 – 530 nm, high photoluminescence quantum yields of ≈100 %, 20 % and 30 % for X = Cl, Br, I respectively and large effective Stokes shifts over 100 nm for all species. Nanocrystals are synthesized by a room temperature, anti-solvent method, but the precursors and ligands are also shown to be effective in a hot injection synthesis. Pure and mixed halide materials show tunable emission by halide concentration with a large FWHM of 80 – 110 nm due to a widely reported exciton self-trapping emission mechanism. Notably, the Cu<sub>3</sub>Cu<sub>2</sub>Cl<sub>5</sub> NCs exhibit a near-unity quantum yield with emission at 520 nm, high crystallinity, and good stability. These materials can be processed and maintained in adequately stable dispersions to enable inkjet printing of these materials into arbitrary patterns. These results indicate that cesium copper chloride NCs may have great potential for future display or lighting applications.

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## **Catalyzed Kinetic Growth in Two-Dimensional MoS<sub>2</sub>**

**City U – Huang Lingli**

**Abstract:** It remains difficult to control the morphology of two-dimensional (2D) materials via direct chemical vapor deposition (CVD) growth. In particular, off-equilibrium (kinetic) growth may produce flakes with non-Wulff shapes (e.g., high-index edges, symmetrical shapes, etc.), which are potentially useful, however a general controllable approach for the kinetic growth of 2D materials are currently lacking. In this work, we pushed the CVD growth of 2D molybdenum disulfide (MoS<sub>2</sub>) into deep kinetic regime, by using potassium chloride (KCl) as catalyst and plasma pretreatment on growth substrates. The unprecedented non-equilibrium high-index faceting and unusual high-symmetry shapes in 2D materials have been realized. The growth mechanism of high-index facets is rationalized based on the theory of kinetic instability on crystal surfaces. This new vapor-liquid-adatom-solid (VLAS) growth mechanism—synergistic capture of multiple vapor phase molecules by the catalyst particles on corners and the oversaturated adatom diffusion along adjacent edges can offer great opportunities for shape engineering on 2D materials. The high-quality, rapid and controllable synthesis of high-index facets (edges) and other non-Wulff shapes of 2D transition metal dichalcogenides will benefit the developments in 2D materials.

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**Ion-Exchange Enabled Artificial Collective Intelligence**

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**Abstract**

The complex system exhibits magnificent collective intelligence, which is contributed by plenty of simple individuals without central command. From the physical point of view, these complexed high order systems are made possible by the strong interaction between active matters, which drive the system far away from its thermodynamic equilibrium. In nature, such nontrivial emergent and self-organizing behaviours are ubiquitously observed in biological systems<sup>1,2</sup>. In principle, the artificial active matters, as the out-of-equilibrium system<sup>3,4</sup>, could also communicate between different species and synergistically enhance their activities, where the bionic ecological system may also be realized. Here we construct a chemical communication system, where the ion-exchange reaction can establish strong coupling between the self-propelled ZnO nanorod and sulfonated polystyrene microbeads (SPSBs), which eventually form an active swarm of the ZnO nanorod-SPSB complex. This synthetic swarm presents some degree of collective intelligence, where the macroscopic phase-segregation and quorum decision-making behavior were observed.

**References**

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**Oral Abstract**

**Highly Steric Congested Arene Borylation: Potential Application in Boron-Containing Polymeric Networks**

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Boron containing polymers are receiving attentions due to its wide range of material applications. Characteristic and application of polymers featuring boroxine linkage are widely investigated recently. The synthesis of these polymers usually involve the dehydration of diboronic acids. However, diboronic acids with good function groups compatibility are difficult to be synthesized using traditional borylation methods. Here we report the first general examples of palladium-catalyzed Miyaura borylation of steric hindered aryl chlorides using the newly developed catalyst system. Nice functional group compatibility was observed under these reaction conditions and the catalyst loading down to 0.05 mol% Pd was able to be achieved for particular entry. Key to success of this reaction relies on the distinctive tailor-made phosphine ligand in which it features of smaller phosphine head and larger remote steric bulk. The arylboronic esters can be attractive building blocks in synthesizing large boroxine network polymers for potential applications in different areas.