confined clusters. Density functional theory calculations revealed that transitions between ferromagnetic and antiferromagnetic states correspond to energies around 1.9–2.0 eV, which match the experimental PL emission near 600 nm. Interestingly, at low dopant levels (< 1%), the PL blue-shifted under magnetic fields, implying magnetic-field-induced destabilization of spin-coupled excitonic recombination. At higher dopant concentrations (~6–7%), excessive spin–spin coupling quenched PL, owing to nonradiative recombination *via* dark exciton states. These results paint a complex but coherent picture: surface ligand chemistry dictates local coordination of the dopant, which in turn governs spin exchange, exciton dynamics, and magneto-optical behavior.

Magnetic measurements performed using a superconducting quantum interference device magnetometer revealed that Mn^{2+}-doped $(CdSe)_{13}$ nanoclusters display paramagnetism with a hint of ferromagnetic hysteresis at 2 K. More astonishingly, the effective magnetic moment reached over 40 μB per cluster at 180 K, vastly exceeding the theoretical spin-only contribution (5.5 μB) of isolated Mn^{2+} ions. The researchers proposed a mechanism involving charge redistribution and spin fluctuations at the Se-rich cluster surfaces. Mulliken population analyses indicated electron transfer from the amine ligands to Se atoms through Cd, creating localized charge imbalances and unpaired spins. These surface states could couple with the Mn^{2+} spins to form magnetic polarons, where charge carriers and localized spins align collectively under internal magnetic fields up to 30 T. Such dynamic spin alignment and electron precession within the clusters explain the enhanced magnetic susceptibility and the emergence of giant magnetic moments. The interplay of ligand chemistry, spin–orbit coupling, and magnetic polaron formation defines a new paradigm for magnetically active nanomaterials that function even at relatively high temperatures. (Reported by Yu-Jong Wu)

This report features the work of Elise Yu-Tzu Li, Yi-Hsin Liu and their collaborators published in Angew. Chem. Int. Ed. ***64****, e202420257 (2025).*

TPS 09A Temporally Coherent X-ray Diffraction
TLS 01C2 X-ray Powder Diffraction
- XRD
- Materials science

TLS 01C1 EXAFS
TLS 17C1 EXAFS
- EXAFS
- Materials sciences

Reference

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Atomic-Level Recycling of a Controversial Herbicide

Through combined experimental and synchrotron analyses, this work reveals the mechanism by which MOF-808 degrades glyphosate and converts it into non-toxic species.

Glyphosate (N-phosphonomethyl glycine; GPh), one of the most widely used herbicides globally, has faced increasing scrutiny for its persistence in ecosystems and potential health impacts. Traditional remediation strategies, such as microbial degradation or oxidation, often transform GPh into equally problematic byproducts like aminomethyl phosphonic acid (AMPA) or phosphoric acid, both of which can be toxic or contribute to eutrophication. The pressing challenge has been to develop a catalytic process that decomposes GPh into truly benign products under mild, environmentally friendly conditions.

A recent study by a collaborative team from the University of New South Wales (Australia), Universidad Nacional de Córdoba (Argentina), Colorado School of Mines (USA), and the NSRRC discovered that Zr-based metal–organic framework nanocrystals (nMOF-808) can completely degrade GPh at room temperature, producing N-formyl glycine and hydroxymethyl phosphonate with very low toxicity.[1] Most remarkably, the reaction proceeds without external energy input and leaves no harmful residues in solution, as the phosphonate byproduct remains bound to the catalyst framework.

MOF-808 is a zirconium-based porous framework consisting of $Zr_6O_4(OH)_4$ clusters connected by benzene-1,3,5-tricarboxylate linkers. Its high stability in water and tunable coordination environment make it ideal for catalytic reactions involving polar molecules. The research team synthesized MOF-808 in two crystal sizes to examine the role of surface defects

and coordinatively unsaturated sites. The nanocrystalline version (nMOF-808) exhibited remarkably enhanced catalytic activity, achieving 95% GPh degradation in just two hours at room temperature, compared to 72% for larger crystals. Nuclear magnetic resonance and mass spectrometry confirmed the production of N-formyl glycine, a benign amino acid derivative, rather than toxic AMPA. Moreover, the catalyst remained effective after multiple reaction cycles, demonstrating robust reusability.

A central question was why the smaller crystals performed considerably better. To address this, the team employed synchrotron-based X-ray absorption spectroscopy (XAS), including extended X-ray absorption fine structure (EXAFS) and near-edge X-ray absorption fine structure. These techniques, performed at the **TPS 44A** quick-scanning XAS beamline of the NSRRC, the Australian Synchrotron, and PETRA III, provided atomic-scale insights into the local coordination environment around the Zr clusters—the catalytic "hot spots" where GPh molecules interact and decompose. EXAFS analyses revealed that at the Zr L_3- and K-edges, the zirconium centers in nMOF-808 have a higher coordination number of labile hydroxyl (–OH) and formate ligands compared to larger MOF-808 crystals. These weakly bound species are key to promoting ligand exchange with GPh, enabling the Cβ–N bond to cleave and drive the degradation reaction, as shown in **Fig. 1**. After catalysis, new scattering paths corresponding to Zr–O–P linkages were observed, confirming that phosphonate fragments become coordinated to the Zr nodes.

Through a synergy of nanostructured catalyst design and state-of-the-art synchrotron spectroscopy, the team demonstrated that zirconium-based MOF-808 nanocrystals can efficiently and selectively degrade GPh into innocuous compounds. The ligand exchange and coordination changes that drive this reaction demonstrate that the path to cleaner chemistry often begins with understanding matter at the atomic scale. This research presents an elegant proof-of-concept for transforming a controversial agrochemical into harmless substances under ambient conditions. The combination of rational catalyst design and synchrotron-enabled structural analysis paves the way for new materials capable of degrading other persistent organic pollutants safely and selectively. Beyond its immediate environmental relevance, the study also demonstrates how *in situ* synchrotron spectroscopy can reveal the dynamic chemistry of MOFs, offering a blueprint for designing next-generation catalysts for green chemistry, water purification, and environmental remediation. (Reported by Yu-Jong Wu)

This report features the work of Alejandro M. Fracaroli, Nicholas M. Bedford and their co-workers published in Angew. Chem. Int. Ed. ***64****, e202424540 (2025).*

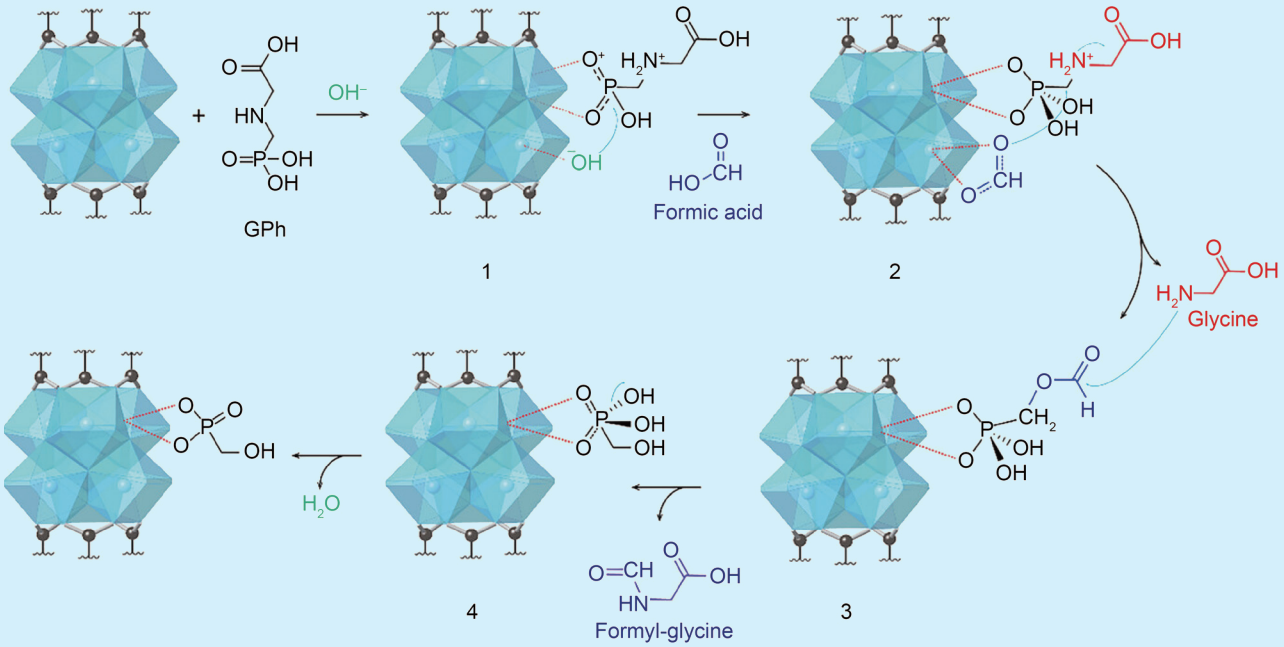

Fig. 1: Proposed degradation mechanism for GPh using MOF-808 as a heterogeneous catalyst. 1) Ligand exchange initiation: GPh's phosphonate group displaces weakly bound formate ligands from the Zr secondary building units, anchoring the molecule to the MOF surface. 2) Cβ–N bond cleavage: hydroxyl groups coordinated to Zr assist a nucleophilic attack on the Cβ atom, breaking the C–N bond to yield glycine and a formyl ester intermediate. 3) Intramolecular formylation: the amine group of glycine reacts with the formyl ester, creating N-formyl glycine. 4) Product trapping and regeneration: the remaining hydroxymethyl phosphonate binds to Zr as a new ligand, while the formate reservoir within the MOF enables multiple reaction cycles. [Reproduced from Ref. 1]

TPS 44A Quick-scanning X-ray Absorption Spectroscopy

- XAS
- Heterogeneous Catalysis, Metal–organic Frameworks

Reference

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How Subtle Atomic Asymmetry Makes Polymers Both Stretchable and Electrically Fast

Through a dipole-tailored polymer design, high stretchability and fast charge transport are achieved for soft, high-performance electronic materials.

Flexible and wearable electronic devices that can stretch, bend, and conform to human skin are rapidly advancing the frontier of biomedical sensing and human–machine interfaces. However, designing polymers that are both mechanically stretchable and electronically conductive has remained a challenge. Typically, increasing flexibility tends to reduce crystalline order, which in turn slows down charge transport. A research team led by Chien-Chung Shih at National Yunlin University of Science and Technology has now addressed this dilemma through smart molecular design. Their study introduces a "dipole-tailoring strategy" that decouples polymer aggregation from crystallinity, allowing a single material to be soft, strong, and electronically agile.[1]

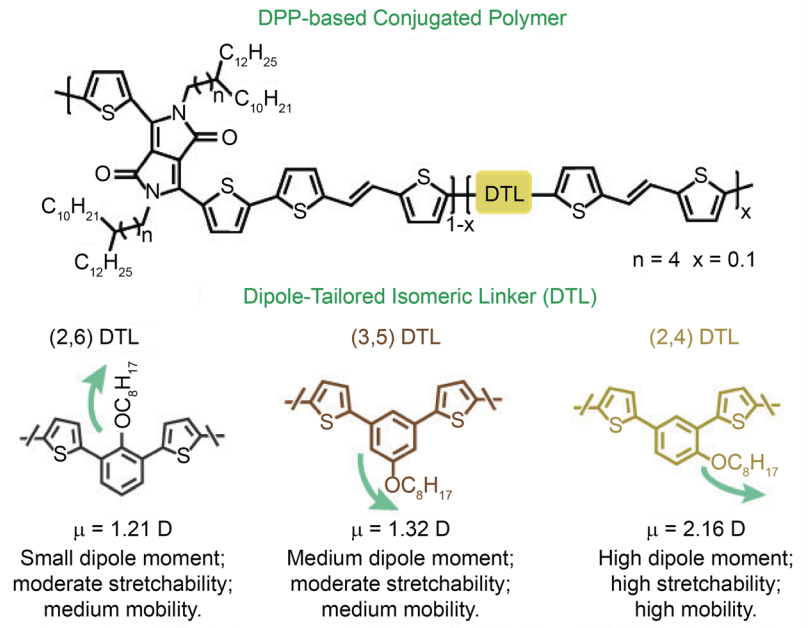

Fig. 1: Chemical structures of the DPP-based conjugated polymers and their isomeric linkers. The parent polymer backbone incorporates a DPP unit and thiophene spacers, while the DTL modulates the local dipole moment through positional variation of the alkoxy substituent on the benzene ring. The three isomers—(2,6)-DTL, (3,5)-DTL, and (2,4)-DTL—exhibit increasing dipole moments (μ = 1.21, 1.32, and 2.16 D, respectively), corresponding to progressively enhanced chain polarity and electrostatic interactions. This dipole engineering enables tunable mechanical and electronic properties: higher dipole moments lead to greater stretchability and improved charge mobility, as demonstrated in the 2,4-DTL polymer. [Reproduced from Ref. 1]

The key innovation lies in dipole-tailored isomeric linkers (DTL) that subtly rearrange the position of an alkoxy group on a benzene ring. By shifting this group from the 2,6- and 3,5- positions to the asymmetric 2,4- position, the researchers created polymers with progressively stronger internal dipoles. This seemingly minor atomic change dramatically reshapes how polymer chains pack, aggregate, and respond to mechanical stress. Through a series of carefully controlled syntheses, the team incorporated each DTL isomer into a diketopyrrolopyrrole (DPP)–thiophene polymer backbone. Spectroscopic and computational analyses showed that the asymmetric 2,4-DTL possesses the highest dipole moment (2.16 D) and the most distorted geometry, thus promoting local electrostatic attraction between chains.

To confirm how these dipolar modifications affect molecular organization, the team relied heavily on synchrotron-based grazing-incidence wide-angle X-ray scattering (GIWAXS) measurements. GIWAXS is uniquely suited to probing the nanometer-scale order