In summary, the study demonstrated that the newly introduced Mo can significantly increase its concentration in wheat grain, posing a potential risk to human health. Identifying Mo species in soils using X-ray absorption spectroscopy provides valuable insight into the roles of soil properties in Mo accumulation in wheat plants. (Reported by Puu-Tai Yang, National Taiwan University)

This report features the work of Puu-Tai Yang and Shang-Li Wang published in J. Environ. Manage. ***374****, 124097 (2025).*

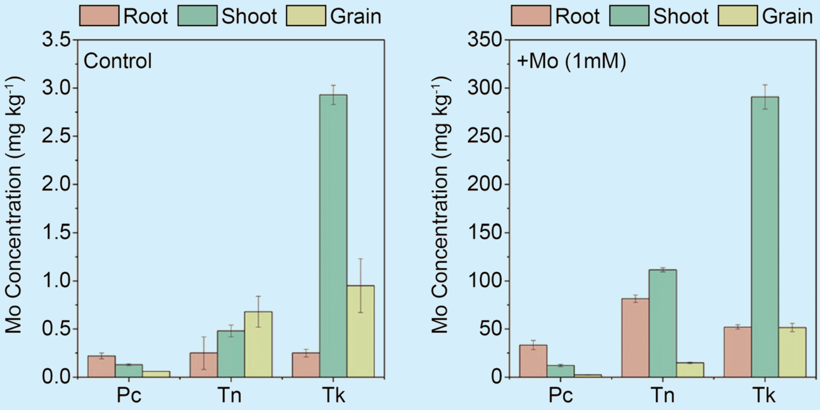

Fig. 2: Mo concentrations in the root, shoot, and grain of wheat plants grown in Pc, Tn, and Tk soils without (control) and with added Mo. [Reproduced from Ref. 2]

TPS 44A Quick-scanning X-ray Absorption Spectroscopy

- XAS
- Environmental Science, Soil Science, Chemistry

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From Atomic Dynamics to Industrial Efficiency: New Pathways for CO_2 Conversion

Catalytic function is governed by atomic-scale motion and interfacial charge control. Synchrotron X-ray techniques reveal both, enabling researchers to connect microscopic dynamics with macroscopic stability.

Carbon dioxide sits at the center of one of humanity's greatest paradoxes. It sustains life by regulating Earth's temperature and feeding plants through photosynthesis—yet in excess, it threatens our climate, our oceans, and our future. As scientists race to build a carbon-neutral world, the ability to transform CO_2 from a waste gas into a renewable feedstock has become a defining challenge of modern chemistry. In the race toward carbon neutrality, two recent breakthroughs, one published in *Nature* and the other in *Journal of the American Chemical Society*, improve our understanding of CO_2 conversion activated by catalysts, from the transient dynamics of single atoms to the structural endurance of industrial-scale alloys. These works led respectively by Hao Ming Chen (National Taiwan University) and Xile Hu (École Polytechnique Fédérale de Lausanne, Switzerland) bridge the gap between atomic-level dynamics and industrial-scale performance. Together, they form a comprehensive view of how catalysts function, adapt, and endure in the fight against climate change.

In the study reported in *Journal of the American Chemical Society*,[1] Chen and his team developed a series of atomically dispersed transition-metal–nitrogen–carbon catalysts (M–N–C), in which individual metal atoms such as Mn, Fe, Co, Ni, or Cu are anchored by nitrogen atoms on a carbon support. Each catalyst consists of metal–nitrogen fourfold sites ($M–N_4$). These materials are widely studied for electrochemical CO_2 reduction, a process that uses electricity to convert CO_2 into carbon monoxide (CO), which can be further processed into fuels or industrial feedstocks. Despite their structural similarity, the catalysts exhibited very different activities. Nickel- and manganese-based M–N–C showed particularly high selectivity and efficiency for CO production, while others were less active. To determine why, the researchers turned to *operando* quick-scanning X-ray absorption spectroscopy performed at **TPS 44A**, which is capable of monitoring the structural evolution of single metal atoms under working electrochemical conditions in real time. The data revealed that the most active catalysts undergo a reversible geometric change during CO_2 reduction. Under applied potential, an extra oxygen atom temporarily coordinates to the metal center, creating a five-coordinate ($M–N_4–O$) configuration. When the potential is removed, the site returns to its original four-coordinate state. This dynamic structural change occurs repeatedly during operation.

Computational analysis showed that this transient coordination affects the electronic structure of the metal, stabilizing a half-occupied dz^2 orbital that promotes CO_2 activation and facilitates CO release. This dynamic site, rather than a static configuration, is responsible for the high catalytic activity, as shown in **Fig. 1**. This finding overturns a common assumption in catalysis that a stable, unchanging structure is always best. Instead, a catalyst's flexibility and ability to reorganize electronically under reaction conditions can be the key to efficiency.

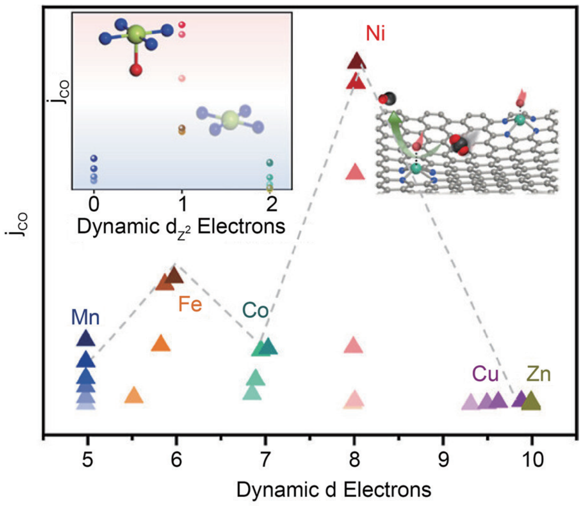

Fig. 1: Correlation between CO production current density (j_{CO}) and the number of dynamic d electrons for atomically dispersed $M–N_4$ catalysts (M = Mn, Fe, Co, Ni, Cu, Zn) during CO_2 electroreduction. Synchrotron-based time-resolved X-ray absorption spectroscopy revealed that the catalytic activity increases with the presence of a half-occupied dynamic dz^2 orbital, which facilitates optimal CO_2 adsorption and CO desorption. Among the series, $Ni–N_4$ exhibits the highest j_{CO} due to its pronounced dynamic dz^2 electron behavior, as illustrated by the inset showing transient structural distortion and CO_2 activation on the $Ni–N_4$ site. [Reproduced from Ref. 1]

While single-atom catalysts operate efficiently at room temperature, industrial CO_2 conversion often takes place under far more extreme conditions, such as in high-temperature solid oxide electrolysis cells. At 800 °C or higher, most materials lose structure or sinter into inactive forms. Achieving both high activity and long-term stability in such environments is a major challenge. In the study published in *Nature*,[2] Hu and his collaborators designed a core–shell nanocatalyst that meets these demands. Their material, composed of a $Co_{0.5}Ni_{0.5}$ alloy core encapsulated by a samarium-doped ceria ($Sm_2O_3–CeO_2$, SDC) shell, was engineered to maintain structural integrity and chemical reactivity during high-temperature operation. The Co–Ni@SDC catalyst exhibited outstanding performance for CO_2 electrolysis, maintaining 90% energy efficiency and 1 A cm^{-2} current density for more than 2,000 hours. This achieves an unprecedented level of durability for such systems. The oxide shell plays several critical roles: it protects the alloy from oxidation, prevents particle agglomeration, and facilitates oxygen ion transport across the interface.

To verify how the material behaves during its long lifetime, the team employed synchrotron X-ray absorption spectroscopy (XAS) measurements at multiple beamlines, including those at NSRRC's **SP 12B1** —the Taiwan-contract beamline

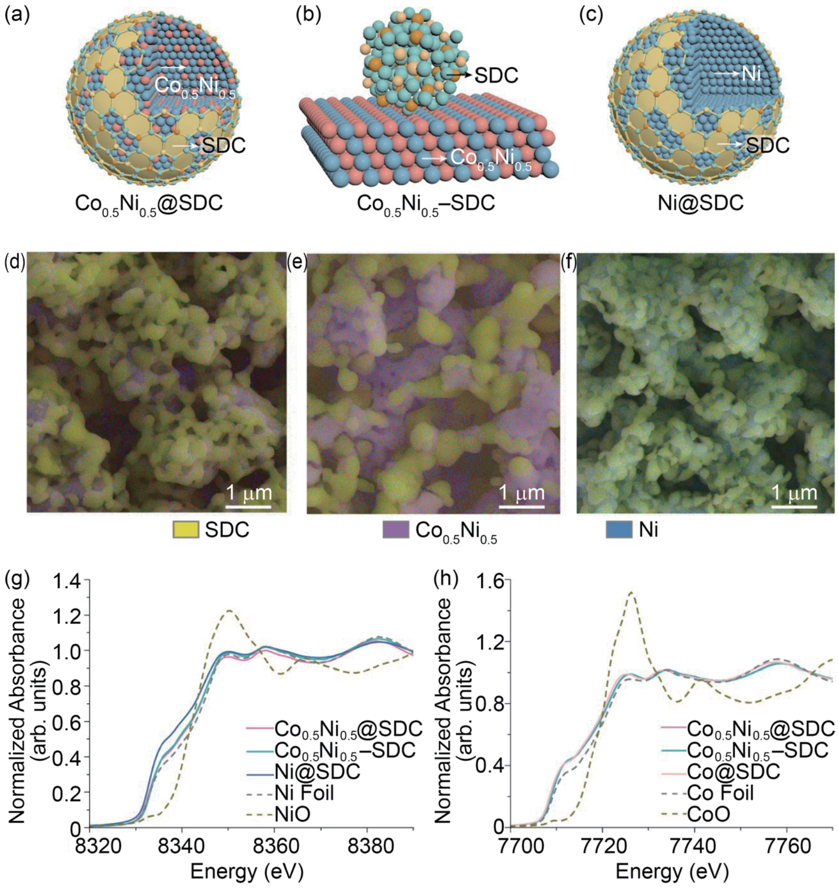

Fig. 2: Schematic illustrations of (a) $Co_{0.5}Ni_{0.5}$@SDC, (b) $Co_{0.5}Ni_{0.5}$–SDC, and (c) Ni@SDC catalysts. Merged scanning electron microscopy and energy-dispersive X-ray spectroscopy mappings for (d) $Co_{0.5}Ni_{0.5}$@SDC, (e) $Co_{0.5}Ni_{0.5}$–SDC, and (f) Ni@SDC catalysts. (g) Ni K-edge XANES spectra and (h) Co K-edge XANES spectra. [Reproduced from Ref. 2]

at SPring-8 in Japan—PETRA III, and the Australian synchrotron. XAS provides detailed information about atomic coordination and electronic states, even under elevated temperatures. The results showed that the alloy core retained its metallic Co–Ni bonding, while the ceria shell remained crystalline and stable, as shown in **Fig. 2**. Crucially, interfacial charge transfer was detected between the metal and the oxide: electrons moved from the Co–Ni core to the CeO_2 lattice, partially reducing Ce^{4+} to Ce^{3+} and creating oxygen vacancies. These vacancies serve as active sites for CO_2 adsorption and activation, while the metallic core promotes electron transfer for CO formation. This dual-site mechanism, verified by *operando* X-ray photoelectron spectroscopy (XPS) and density functional theory calculations, explains both the catalyst's high activity and its resistance to degradation. The interface acts as a self-regulating system, continuously balancing charge and maintaining structural stability under harsh conditions.

Although the above-mentioned studies focus on different systems, they tell a consistent story about how CO_2 conversion can be optimized. In both cases, the key lies in understanding the relationship between structure, electronic behavior, and reaction environment, and synchrotron X-rays make that understanding possible. At the atomic scale, X-ray spectroscopy revealed that catalytic activity emerges from the dynamic adaptation of electronic orbitals during reaction. At the macroscopic scale, high-energy X-ray and XPS analyses demonstrate that long-term durability arises from controlled charge transfer across interfaces. Together, these insights form a continuous picture of how catalysts must behave: responsive enough to activate CO_2 efficiently, yet stable enough to operate for thousands of hours. Furthermore, both studies highlight the growing importance of *operando* (*in situ*, under working conditions) measurements. Traditional "before-and-after" characterization provides only static images, missing the transient phenomena that govern real catalytic behavior. Synchrotron radiation, with its intense and tunable X-rays, allows scientists to collect structural and electronic information directly during reaction, bridging the gap between laboratory design and practical performance.

Overall, these findings redefine how researchers design materials for CO_2 utilization. In low-temperature electrochemical systems, understanding dynamic orbital behavior helps identify active configurations and design catalysts that can adapt under applied potentials. In high-temperature systems, insights into interfacial charge flow and oxygen vacancy formation enable the creation of long-lasting reactors suitable for industrial deployment. The implications extend beyond CO_2 conversion. The same principles are applicable to water splitting, ammonia synthesis, hydrocarbon reforming, and any reaction in which the interplay between electrons, atoms, and surfaces determines efficiency. The combined use of synchrotron spectroscopy, theoretical modeling, and materials engineering is now recognized as a cornerstone of modern catalysis research. (Reported by Yu-Jong Wu)

This report features the works of Hao Ming Chen, Xile Hu, and their collaborators published in J. Am. Chem. Soc. ***147****, 13027 (2025) and Nature* ***641****, 1156 (2025).*

TPS 44A Quick-scanning X-ray Absorption Spectroscopy
SP 12B1 Materials X-ray Study

- XAS
- Materials Science

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