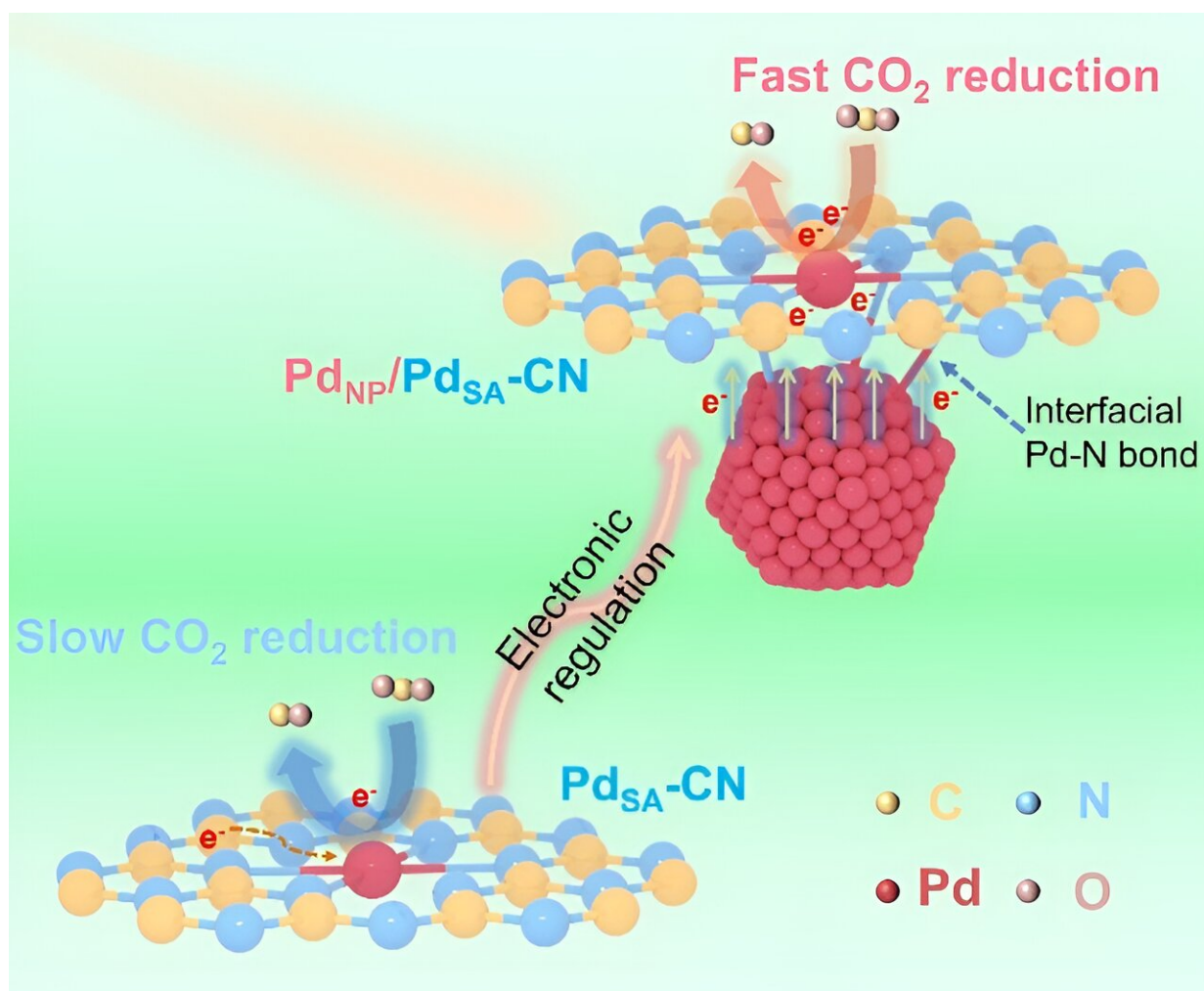


# Synergy palladium single atoms and twinned nanoparticles for efficient CO<sub>2</sub> photoreduction

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Schematic diagram of CO<sub>2</sub> photoreduction mechanism. Credit: Lei, Li et al.,

The challenge of regulating the electronic structures of metal single-atoms (M-SAs) with metal nanoparticles (M-NPs) lies in the synthesis of a definite architecture. Such a structure has strong electronic metal-support interactions and maintains electron transport channels to facilitate carbon dioxide photoreduction (CO<sub>2</sub>PR).

In a study [published](#) in *Advanced Powder Materials*, a group of researchers from Zhejiang Normal University, Zhejiang A&F University and Dalian University of Technology, revealed the engineering of the [electron density](#) of Pd single atoms with twinned Pd nanoparticles assisted by strong electronic interaction of the atomic metal with the support and unveiled the underlying mechanism for expedited CO<sub>2</sub>PR.

"As one of the most promising CO<sub>2</sub>PR semiconductors, polymeric graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) featured with sp<sup>2</sup> π-conjugated lamellar structures can offer electronegative nitrogen atoms to anchor M-SAs, forming active metal-nitrogen moieties (M–N<sub>x</sub>)," explained Lei Li, lead author of the study. "However, stable M–N<sub>x</sub> configurations forbid tunability of electronic structures of M-SA sites."

In particular, the extent of d-states of transition metals relative to Fermi level dictate metal–adsorbate binding strengths, which should be neither too weak nor too strong for the optimal catalytic activity. Thus, precise tailoring of electronic structures for metal centers is essential for efficient and selective CO<sub>2</sub>PR.

"Loading M-NPs on the hosts can be applied in modifying the metal single-sites without sacrificing pristine properties. Additionally, considering the high electron density of M-NPs, it is highly probable that charge density rearrangement occurs between M-SAs and M-NPs connected through ligand bridges," added Yong Hu, col-lead and co-corresponding author. "However, electronic interactions of M-SAs with M-NPs synchronously coordinated on g-C<sub>3</sub>N<sub>4</sub> are rarely exploited in

photocatalytic applications."

The researchers also found that the electronegative N sites in g-C<sub>3</sub>N<sub>4</sub> bridged Pd-SAs and Pd-TPs, forming Pd–N bonds to create strong electronic metal-support interactions and permitting directional electron transport from Pd-TPs to Pd-SA sites for effective CO<sub>2</sub>PR.

Both experimental and [theoretical studies](#) confirmed the multiple roles of Pd-TPs. The Pd-TPs served as an electron donator to enrich electron density on catalytic centers of single-Pd-sites through N ligands in g-C<sub>3</sub>N<sub>4</sub> networks, thereby down-shifting the d-band center to accelerate carbonyl desorption for CO production.

The team's findings offer a feasible approach to maneuver electronic structures of neighboring metal single sites by integrating [metal nanoparticles](#) for photocatalysis.

**More information:** Lei Li et al, Electron-enriched single-Pd-sites on g-C<sub>3</sub>N<sub>4</sub> nanosheets achieved by in-situ anchoring twinned Pd nanoparticles for efficient CO<sub>2</sub> photoreduction, *Advanced Powder Materials* (2024). [DOI: 10.1016/j.apmate.2024.100170](https://doi.org/10.1016/j.apmate.2024.100170)

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