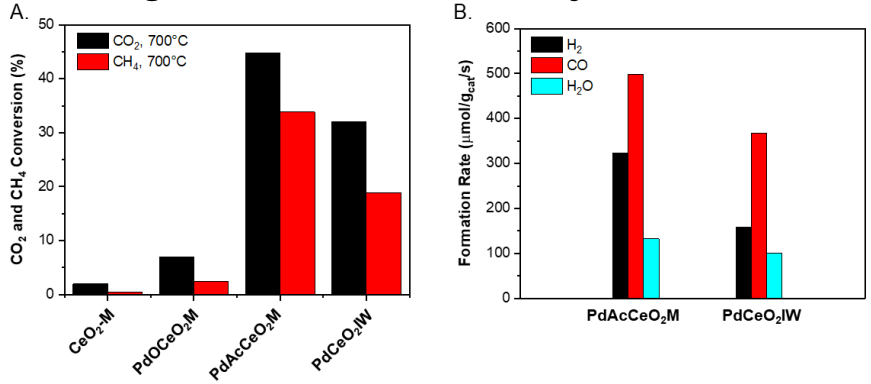
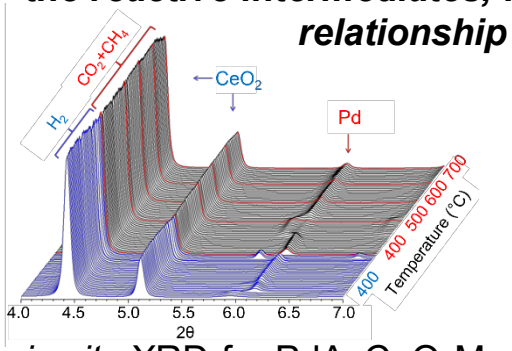
# Unraveling Mechanism of Methane Dry Reforming over Mechano-Chemically prepared $Pd/CeO_2$

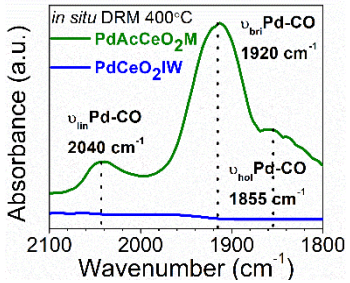
***Mechano-chemically prepared $PdAcCeO_2M$ show selective pathways toward hydrogen production using an efficient, scalable synthesis method***




***In situ XRD reveals presence of unique Pd structure in $PdAcCeO_2M$, where DRIFTS captures nature of the reactive intermediates, linking structure-surface relationship for DRM***




*in situ* XRD for $PdAcCeO_2M$




*in situ* DRIFTS

## Scientific Achievement:

Ball milled $PdAcCeO_2M$ shows a unique methane dry reforming reaction mechanism with improved chemistry over wet chemical synthesis methods. Scientists from Brookhaven National Laboratory and the Universita de Udine (Italy) collaborated to discover the reaction mechanism for methane dry reforming at the limits of experimental detection.

## Significance and Impact:

Determining the precise role of $CO_2$ and $CH_4$ during methane dry reforming allows for the development of novel catalysts formulations. Via isotopically labelling the mechanism, the contributions from each reactant was isolated to reveal a rich surface chemistry.

## Research Details:

- Mechano-chemically prepared $PdAcCeO_2M$, which uses a facile and scalable synthesis, showed increased DRM reactivity relative to standard $PdCeO_2IW$
- in-situ techniques including IR, AP-XPS and XAS revealed nature of the active site: $Pd^0$-$C_x$ sites near $Ce^{4+/3+}$. CO and HCOO via $CO_2$ reduction was key to the proposed mechanism.
- DFT calculation align with experimental findings, suggesting the formation of Pd-$C_x$ intermediates as a preferential Pd structure for adsorption of CO


Jimenez, J.D.†, Betancourt, L.E.†, Danielis, M., Zhang, H., Zhang, G., Orozco, I., Xu, W., Llorca, J., Liu, P., Trovarelli, A., Rodriguez, J.A., Colussi, S.*, Senanayake, S.D.* *ACS Catalysis*. 2022, 12,12809–12822


**Front Cover; Featured Article**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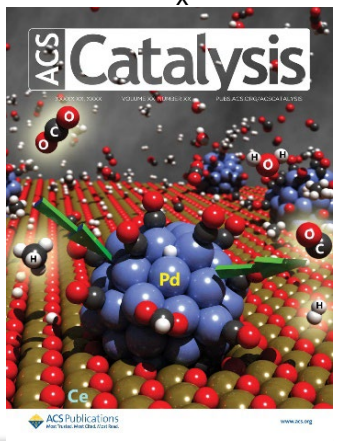



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