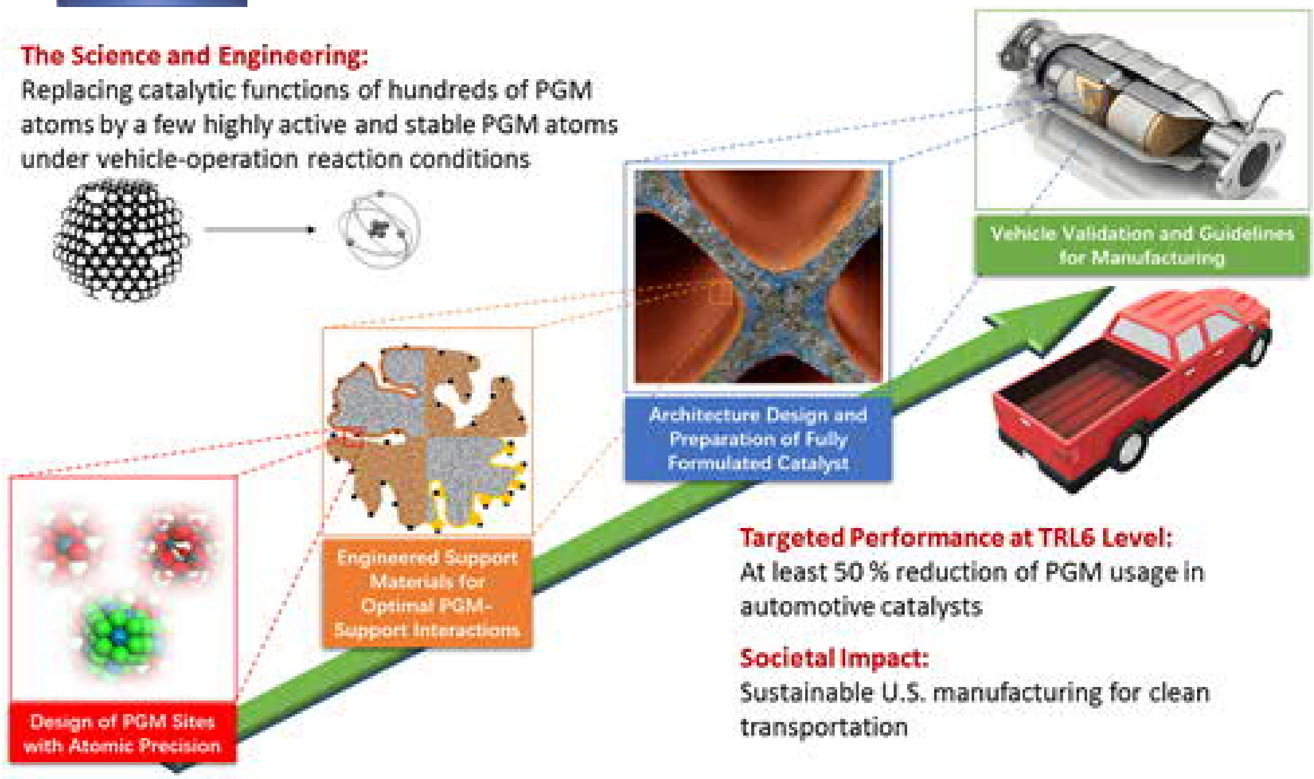
Project Title: Slashing PGM in Catalytic Converters: An Atoms-to-Autos Approach

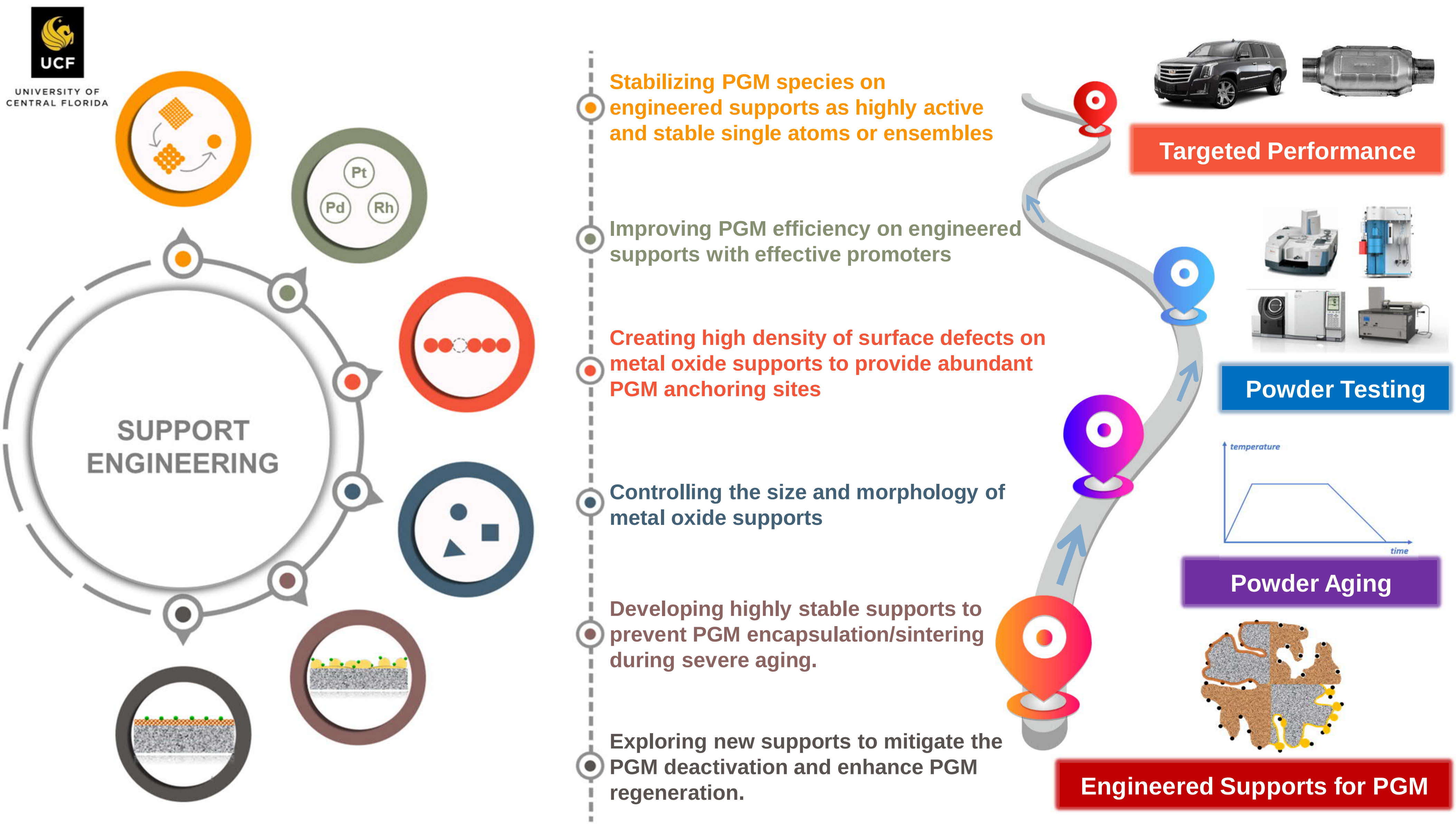
<u>Proposed Objectives:</u>

- enable new three-way catalyst technologies to reduce PGM use in the US gasoline vehicle fleet by 50%

<u>Project Impact/Takeaway:</u>

- Develop new PGM catalyst concepts with near 100% utilization efficiency and excellent activity and durability
- Significantly reduce the PGM use in automotive catalysts to mitigate the supply/demand imbalance





UCF
UNIVERSITY OF CENTRAL FLORIDA
SUPPORT ENGINEERING
Pt
Pd
Rh
Stabilizing PGM species on engineered supports as highly active and stable single atoms or ensembles
Improving PGM efficiency on engineered supports with effective promoters
Creating high density of surface defects on metal oxide supports to provide abundant PGM anchoring sites
Controlling the size and morphology of metal oxide supports
Developing highly stable supports to prevent PGM encapsulation/sintering during severe aging.
Exploring new supports to mitigate the PGM deactivation and enhance PGM regeneration.
Targeted Performance
Powder Testing
temperature
time
Powder Aging
Engineered Supports for PGM

Kinetic analysis pre and post degradation

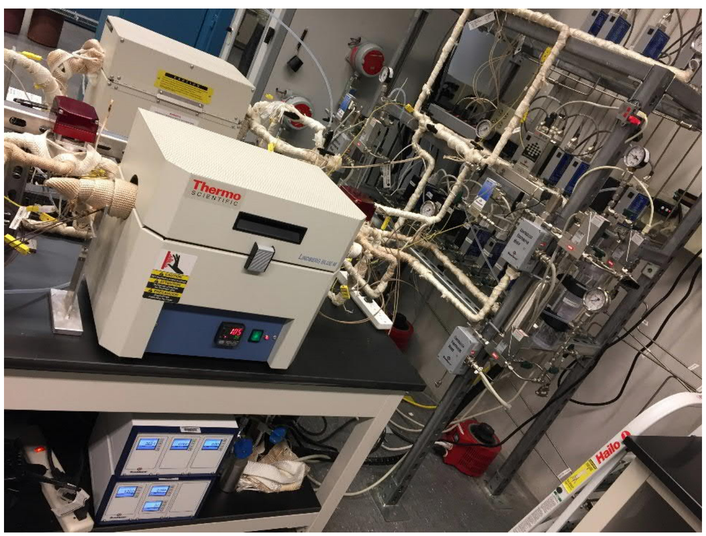
Rate, activation energy and reaction order analysis

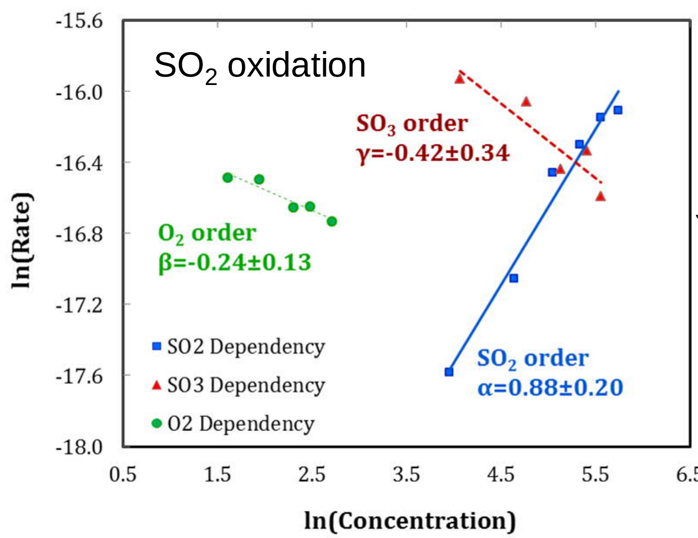
Includes active site characterization and quantification

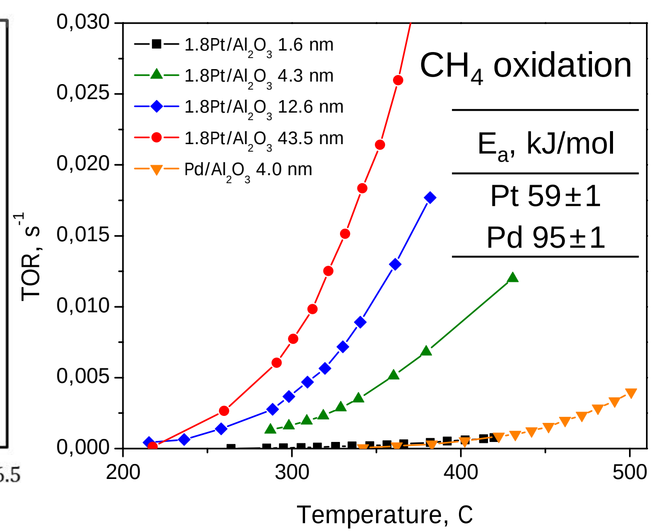
HC and CO oxidation over new and baseline Pd-based materials
NOx reduction over new and baseline Rh-based materials

Degradation → lean/rich cycling protocols

Rate analysis with integrated Pd/Rh system



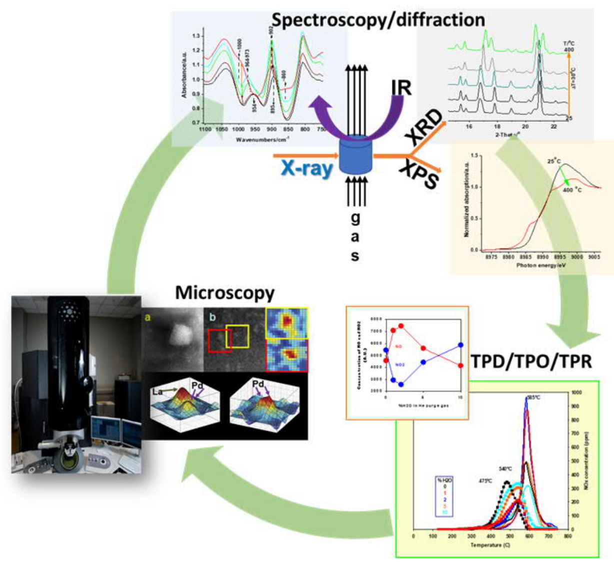




PNNL Capabilities

IR

- Static transmission FTIR with mass spec with precise temperature (-180 to 900 ºC) and pressure control (10^{-8} to 10^{3} Torr)
- DRIFTS under relevant flows and reaction temperatures (<500 ºC)
- *Nature and structure of adsorbates; provides insight to size, structure, chemical state of active metal components in TWC.*



XPS

- High energy resolution spectra collected using a pass-energy of 69.0 eV with a step size of 0.125 eV, coupled with custom-built gas manifolds and gloveboxes. Catalysts can be treated with various gases and gas mixtures without their removal from the XPS cell at temperatures up to 1100 ºC (quasi *in situ*).
- *Provides information on oxidation state of Pd/Rh/Ce and the surface content of the relevant catalytically-active species.*

XRD

- High-resolution *ex situ* and *in situ* X-ray diffraction (XRD)
- *XRD can observe metal Pd or PdO nanoparticles and estimate their average size*
- *In-situ XRD can monitor crystallographic changes in alumina, ceria and CZO supports during heat treatment*

Microscopy

- **HAADF-STEM** (high-angle dark field scanning transmission electron microscopy) and **ETEM** (environmental TEM); allows the observation of nanomaterials *in situ*) studies on a FEI Titan 80-300 electron microscope, equipped with a HAADF detector.
- *Can observe metal nanoclusters in the absence or presence of reactants to probe changes in structure during catalysis.*

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Transforming advance powder materials to full-size monolith catalysts

- Powder material scale-up
  - Material discovery with scalability in mind
  - Scaling up material with minimum activity loss
- Slurry chemistry and catalyst design
  - Optimizing slurry chemistry and rheology for new materials
  - Adopting advanced slurry coating processes
  - Developing customized catalyst designs for a benchmark engine
- Performance validation
  - Reactor testing with monolith sample cores to validate material performance
  - Engine and vehicle testing to evaluate full-size catalyst performance