Joint Development and Coordination of Emissions Control Data and Models (CLEERS Analysis & Coordination)
Project ID: ACE022

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Annual Merit Review

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This presentation does not contain any proprietary, confidential, or otherwise restricted information

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  - Haiying Chen
- **Guidance from CLEERS Advisory Committee members:**
  - Wei Li, Christine Lambert, Craig Dimaggio, Mike Cunningham, John Kirwan, Louise Olsson, Mike Harold, Stuart Daw
- **Collaboration with partners at PNNL:**
  - Mark Stewart, Ken Rappé, Yong Wang, Jamie Holladay

Overview

Timeline

Project start date: FY2019

Project end date: FY2021

- part of ORNL response to 2018 VTO "Lab Call"
- core activity since FY2000
- supports and coordinates emissions control research
- evolves with DOE priorities and industry needs

Budget

	FY18	FY19
Coordination	$250k	$250k
Analysis	$325k	$450k

Barriers

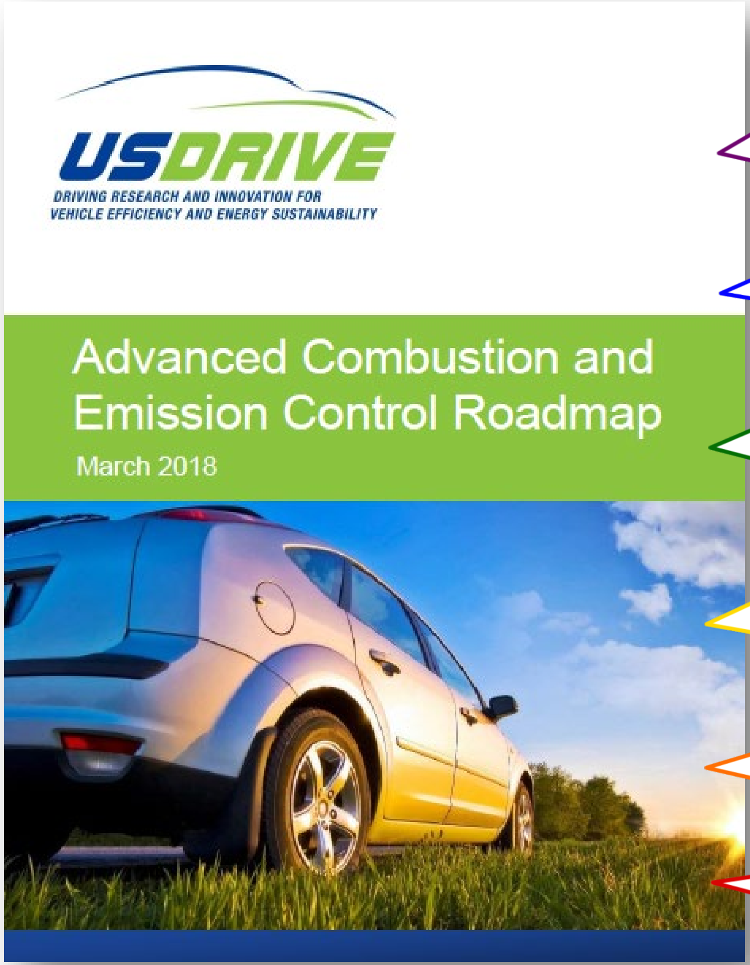
U.S. DRIVE Advanced Combustion & Emission Control 2018 Roadmap Barriers & Targets:

- U.S. EPA Tier 3 Bin 30 emission standard
- 90% conversion of criteria pollutants (NOx, CO, HCs) at 150°C for the full useful life of the vehicle
- "Development of models and simulation tools… to predict performance and better understand catalytic processes"

Partners

- DOE Advanced Engine Crosscut Team
- University of Virginia, Johnson Matthey, PNNL
- U.S.DRIVE ACEC Tech Team
- CLEERS Focus Group members:
  - 10 engine/vehicle manufacturers
  - 9 component and software suppliers
  - 12 universities
  - 4 national labs

U.S. DRIVE ACEC Roadmap emphasizes the need for advanced aftertreatment research to ensure emissions compliance for high efficiency combustion engines



"Compliance with exhaust emission regulations will be mandated and requires aftertreatment technologies integrated with the engine combustion approaches."

"The overarching emissions goal… is the U.S. EPA Tier 3 Bin 30 emission standard…"

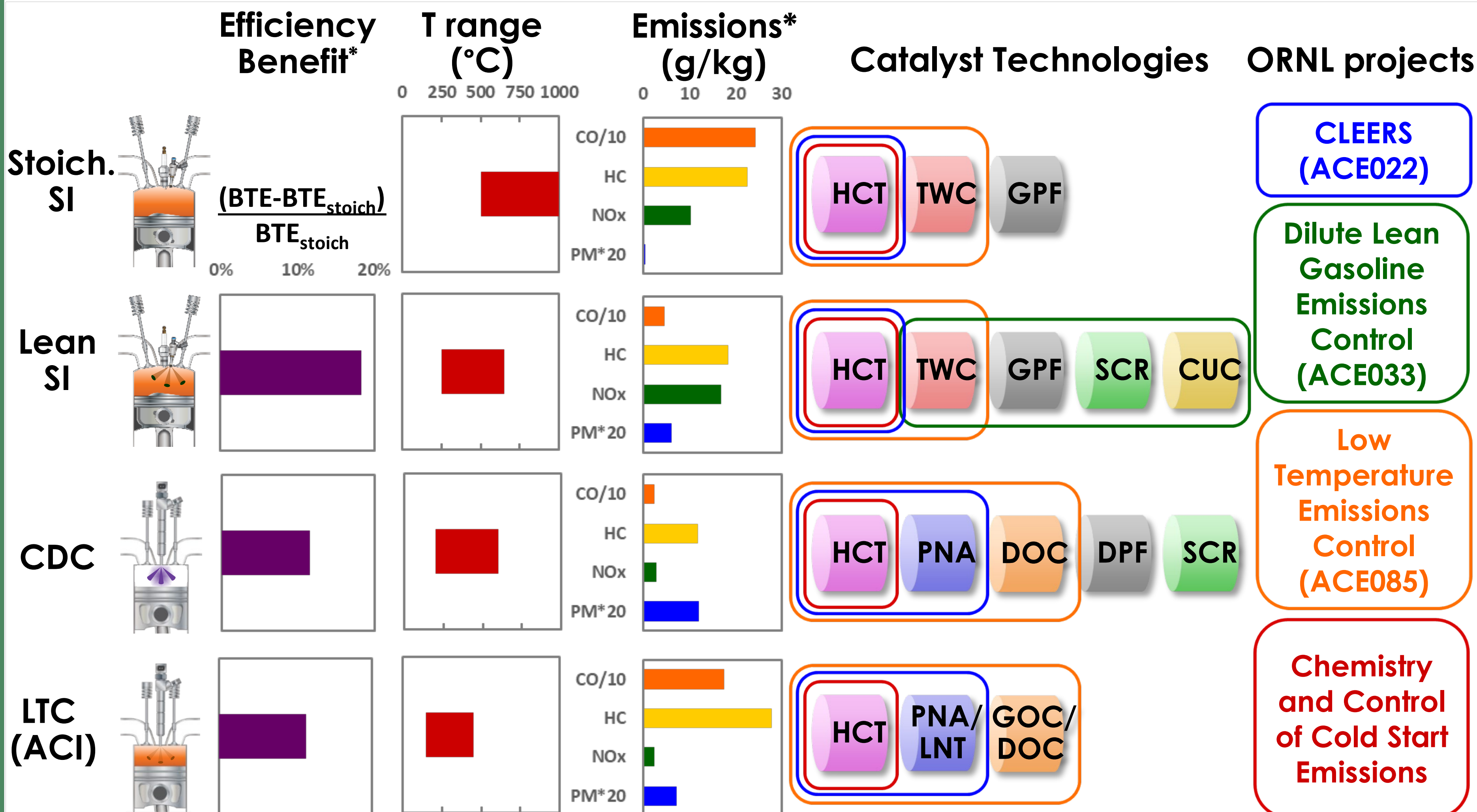
"…achieve greater than 90% conversion of criteria pollutants (NOx, CO, HCs) at 150°C for the full useful life of the vehicle."

"…development of models and simulation tools ranging from the molecular level to the system level to predict performance and better understand catalytic processes"

"Understand the state of the PNA/HC Trap for shutdown /restart optimize restart/cold start performance"

"Characterize and understand PNA/HC Trap durability"

Advanced engines improve efficiency, but lean low temperature exhaust creates emissions challenges that must be addressed



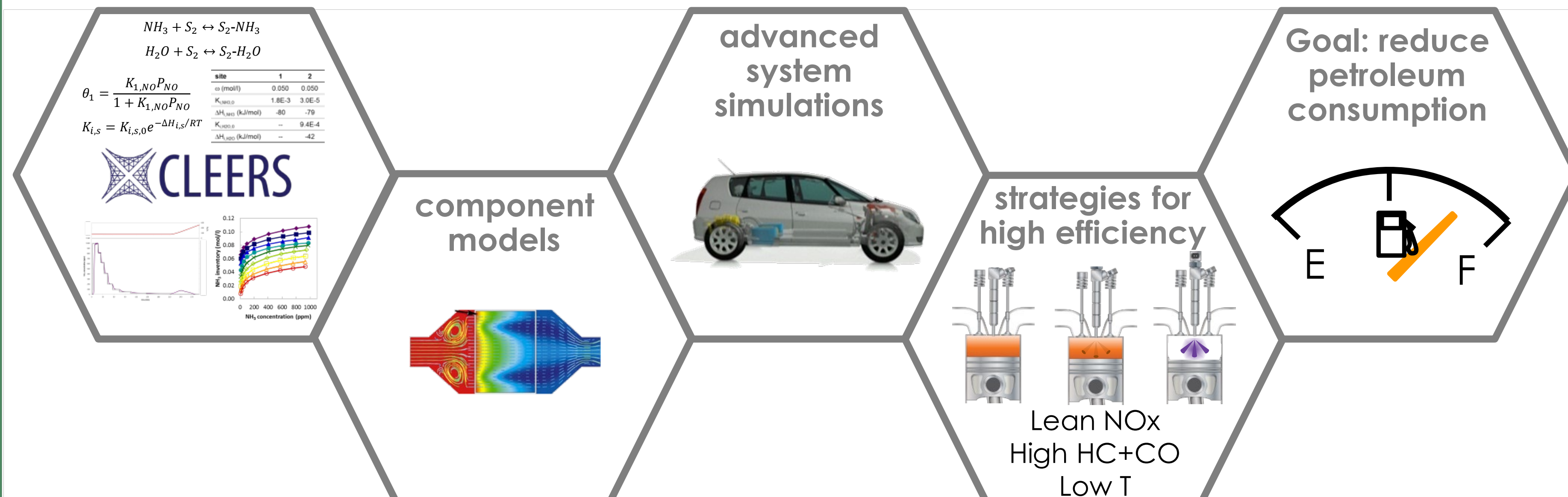
*(efficiency and emissions at 2000 rpm, ~2 bar BMEP)

CLEERS provides a key stepping stone on the path to reduced petroleum consumption

- CLEERS = **C**rosscut **L**ean (/**L**ow-temperature) **E**xhaust **E**missions **R**eduction **S**imulations

- Mission: accelerate development of emissions control technologies for high efficiency advanced combustion engines by improving accuracy of aftertreatment system simulations

- Objectives:
  - develop and disseminate pre-competitive data, parameters, and models
  - support collaborations among industry, university, national lab partners
  - gather feedback from industry on critical emissions control research needs
  - coordinate DOE National Laboratory research efforts



ORNL coordinates CLEERS activities and conducts focused R&D in support of CLEERS objectives

ORNL CLEERS Coordination **ORNL CLEERS Analysis**

Pacific Northwest NATIONAL LABORATORY

*= collaboration with PNNL

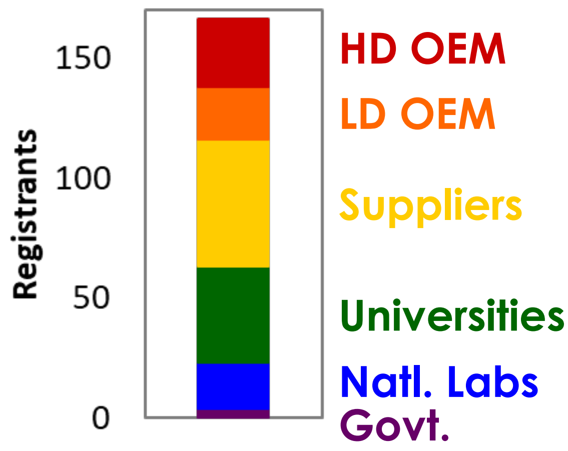
Milestones

FY	Qtr	Milestone	Status
2018	4	Organize 2018 CLEERS Workshop	complete
2019	4	Publish/present model for NO adsorption and release on a Pd-zeolite PNA	on schedule
2019	4	Organize 2019 CLEERS Workshop	on schedule

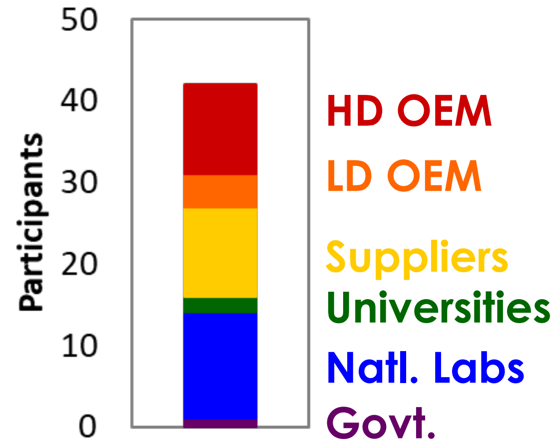
CLEERS is an efficient means for communicating pre-competitive information across the emissions control community

- Workshop #21, Sep 18-20, 2018, Ann Arbor, MI
  - 166 attendees representing OEMs, component & software suppliers, national labs, universities, government agencies
  - 39 presentations (4 invited), 24 posters
  - Panel discussion on emissions control challenges and opportunities for hybrid vehicles
  - Proceedings in special issue of Emission Control Science & Technology
- Focus Group teleconferences:
  - Technical presentations of latest results
  - 40-60 invited participants from around the world
  - >50% industry representatives

2019 CLEERS Workshop Registrants



March 2019 CLEERS Focus Group Teleconference Participation



Supported the U.S.DRIVE ACEC LTAT team in developing and testing experimental protocols for low temperature catalysts

U.S.DRIVE
ACEC Tech Team
Low Temperature Aftertreatment Working Group

Org.	Representatives
FCA	Craig DiMaggio Vence Easterling
Ford	Joe Theis
GM	Se Oh Ming Yang
PNNL	Ken Rappe Mark Stewart
ORNL	Josh Pihl Todd Toops
UM	Galen Fisher
DOE	Ken Howden


Aftertreatment Protocols for Catalyst Characterization and Performance Evaluation:
Low-Temperature NH_3-SCR Catalyst Test Protocol

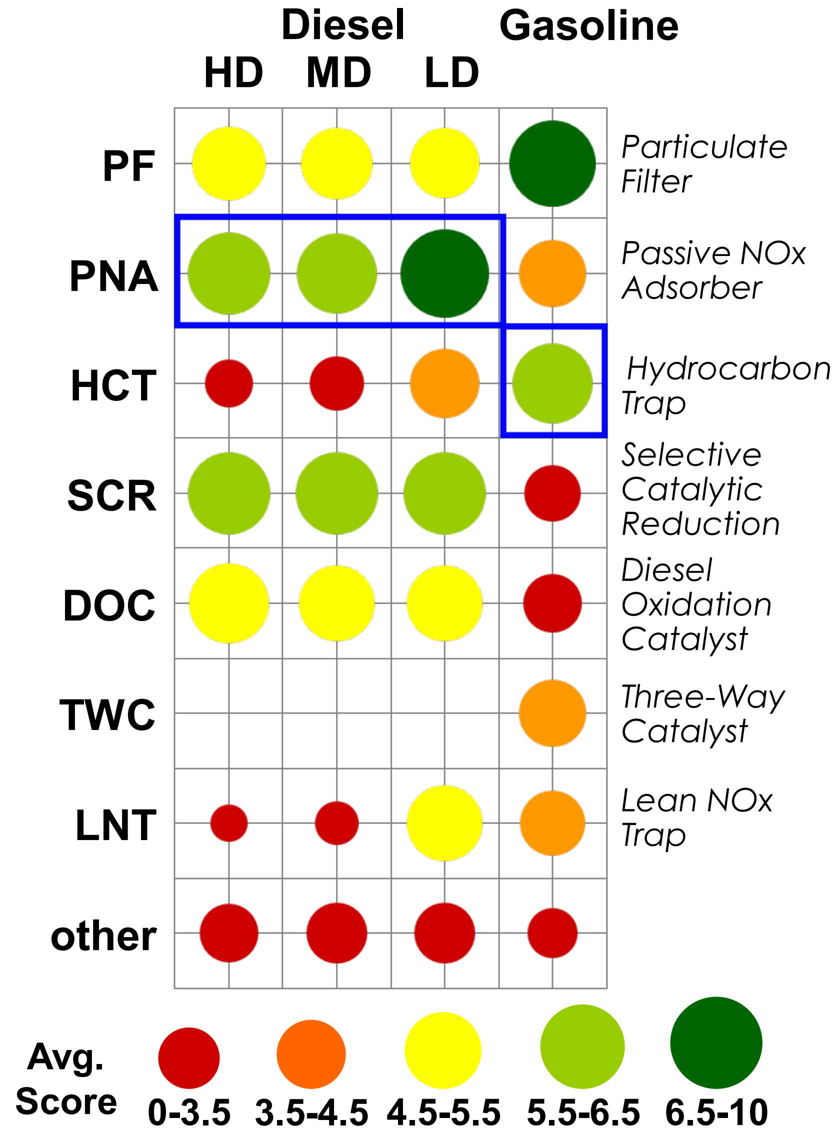
The Advanced Combustion and Emission Control (ACEC) Technical Team
Low-Temperature Aftertreatment Group

March 2019

- Supported development of low T catalyst screening protocols for oxidation (2014-15), NOx+HC storage (2015-18), TWCs (2016-17), and NH_3 SCR (2018)
  - Forthcoming summary journal publication in ECS&T
- Hosting protocols on CLEERS website

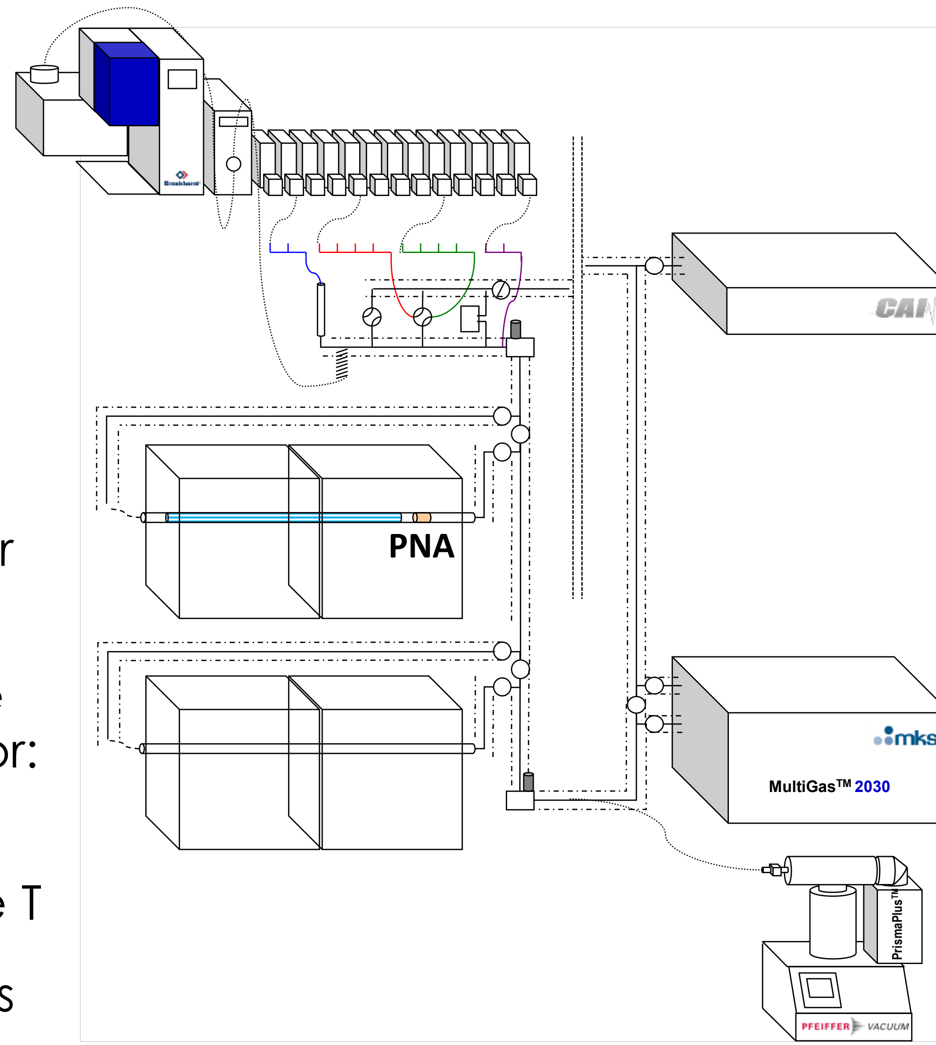
2017 CLEERS Industry Priorities Survey showed continuing interest in low temperature strategies

- Participants asked to rank dozens of potential R&D topics as high, medium, or low priority
- Top ranked technologies varied by application:
  - gasoline: GPFs, HC traps
  - diesel: PNAs, urea SCR
- ORNL's CLEERS R&D activities are currently focused on understanding and modeling the operation and aging of:
  - passive NOx adsorbers (PNA)
  - hydrocarbon traps (HCT)

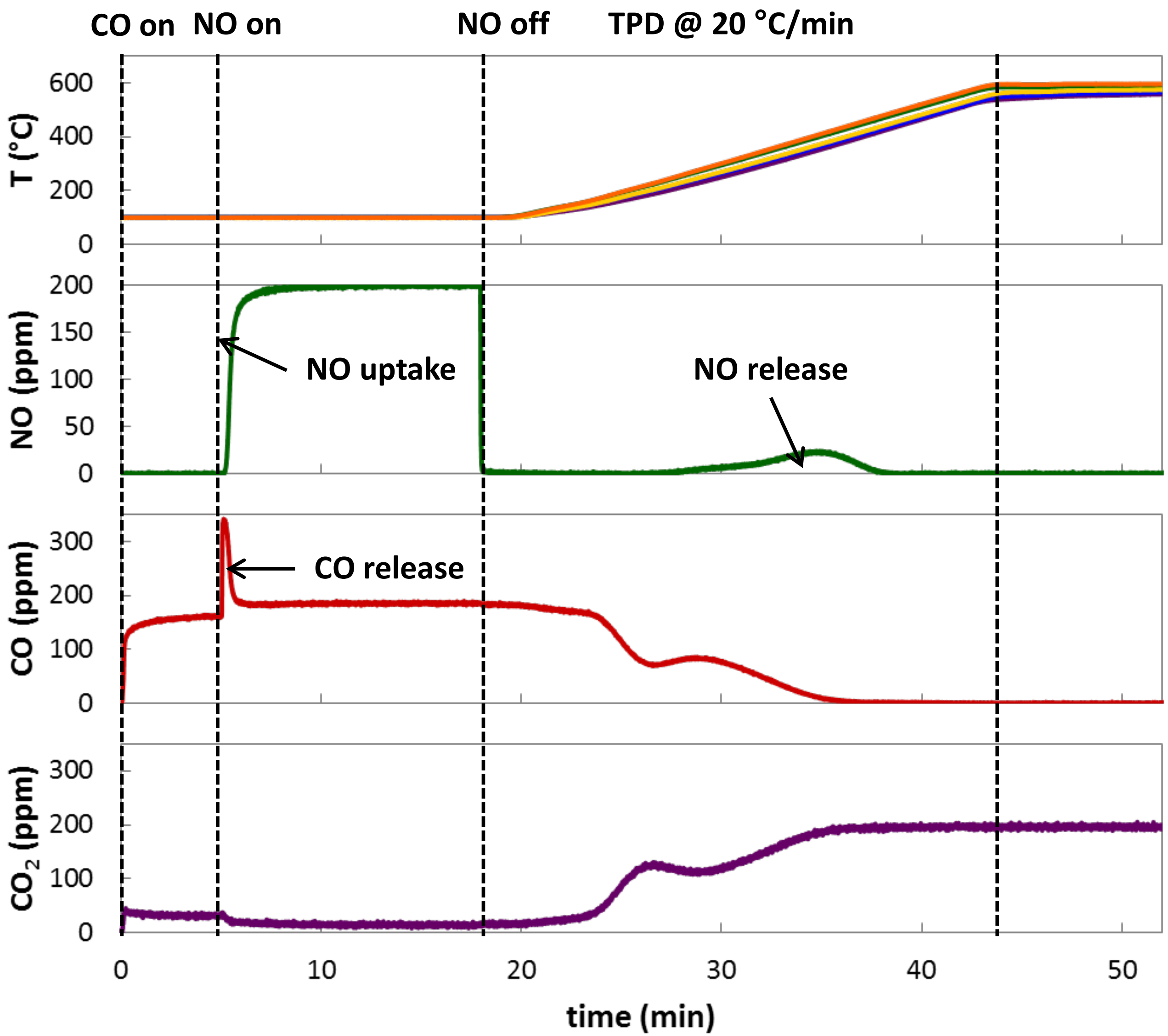


Used synthetic exhaust flow reactor and DRIFTS experiments to reveal the chemistry underlying NO adsorption on a PNA

- Obtained catalyst core sample from Johnson Matthey
  - model dCSC™ component
  - Pd-exchanged ZSM-5
    - Pd loading: 50 g/ft^3 (1.8 g/l)
  - washcoated on a 400 cells/in^2 cordierite monolith
- Degreened at 600 °C for 4 h under 10% O_2/7% H_2O/N_2
- Measured NO uptake and release on a synthetic exhaust flow reactor:
  - isothermal NO adsorption/TPD
  - varied concentrations, storage T
- Investigated surface intermediates with DRIFTS



PNA isothermal storage/TPD experiments enable reproducible measurements of capacity and stability

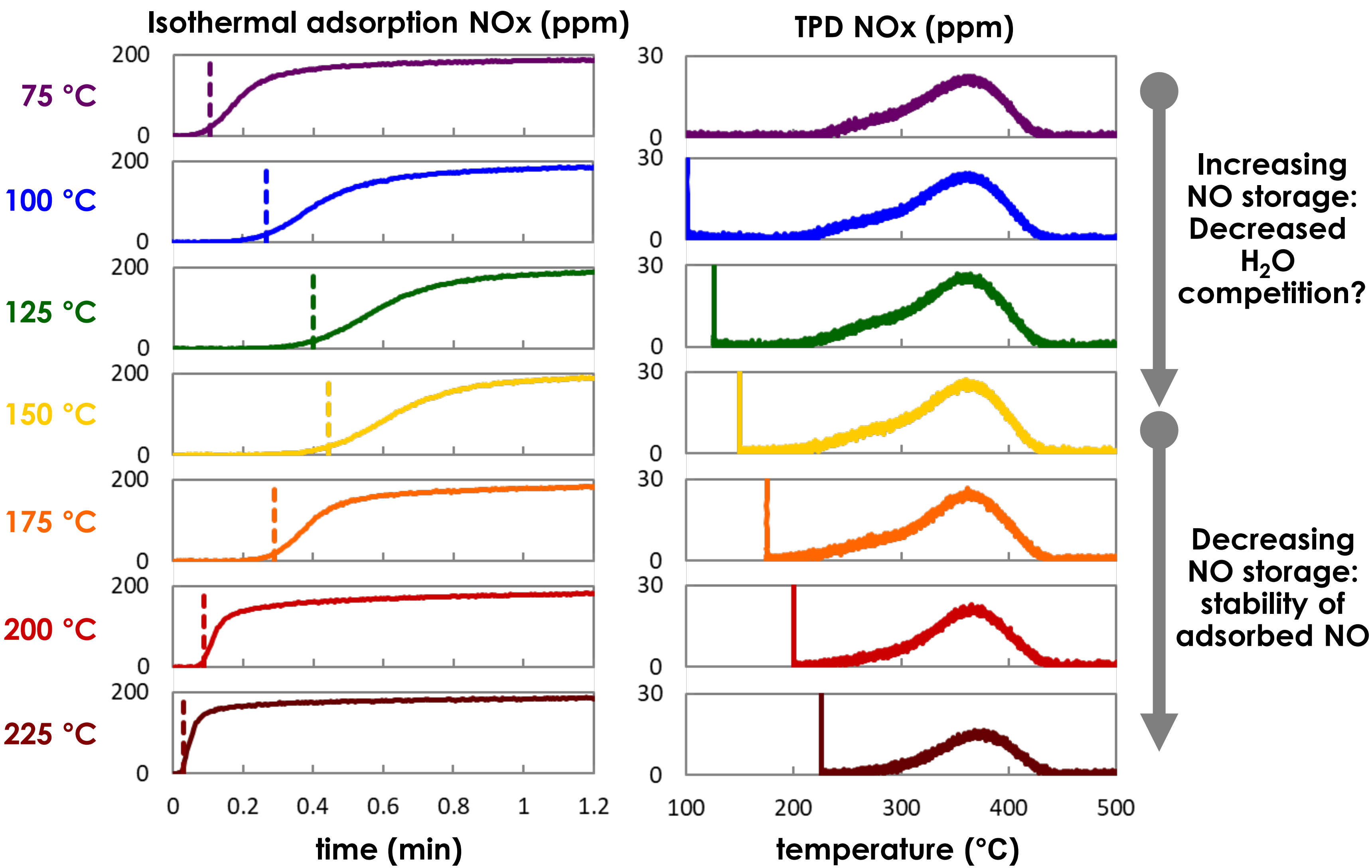


pretreat, cool conditions	
O_2	10%
H_2O	7%
T	600-100°C
SV	30000 h^{-1}

NO exposure conditions		
NO	200 ppm	(25-1600)
CO	200 ppm	(50-800)
O_2	10%	(1-13)
H_2O	7%	(5-13)
CO_2	0%	(0-13)
T	100°C	(75-225)
SV	30000 h^{-1}	

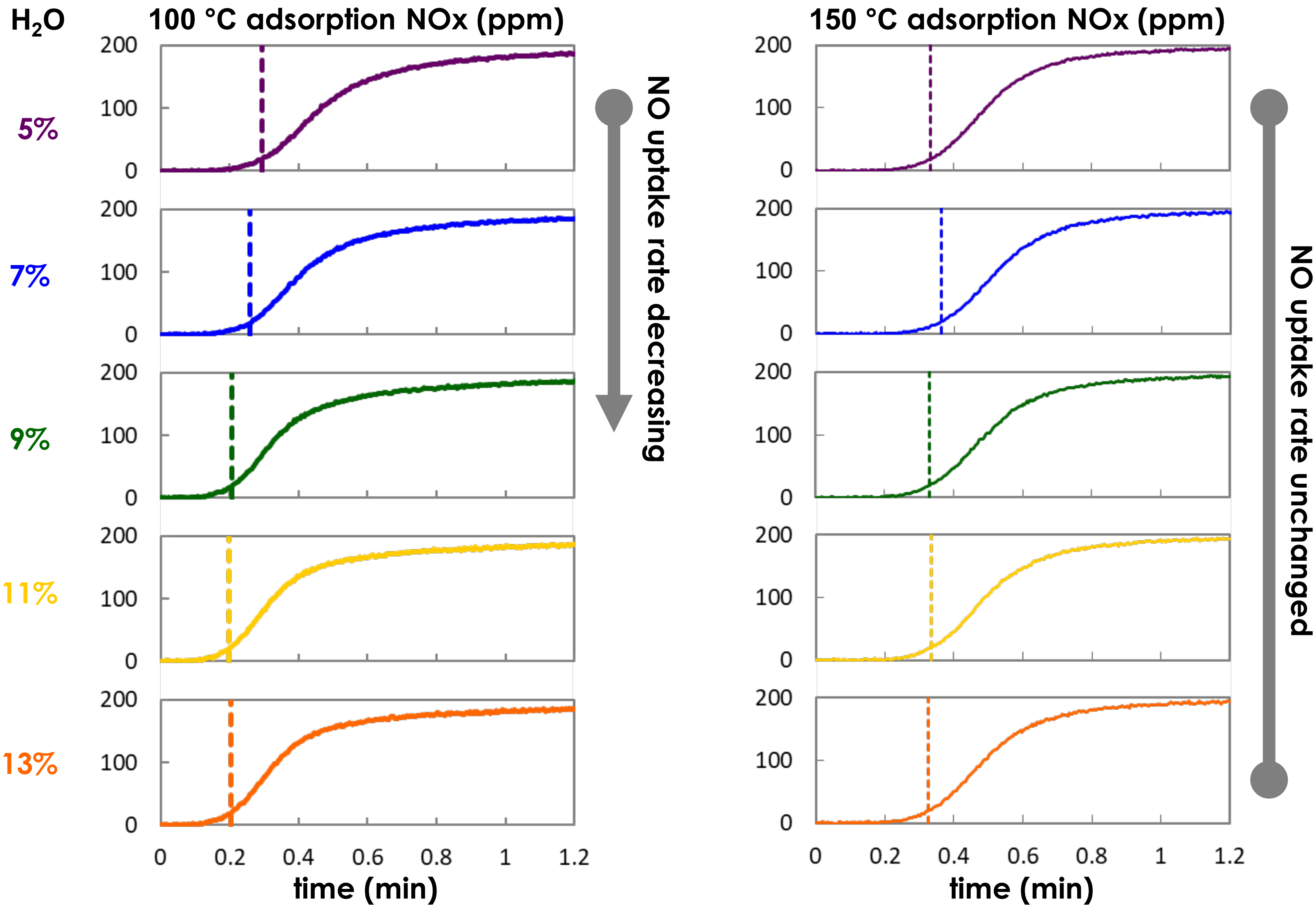
Note: procedure focuses on reaction mechanism identification and model parameter estimation, and therefore differs from the ACEC LTAT protocol for storage catalyst performance evaluation

NO uptake initially increases with adsorption temperature, then decreases[1]



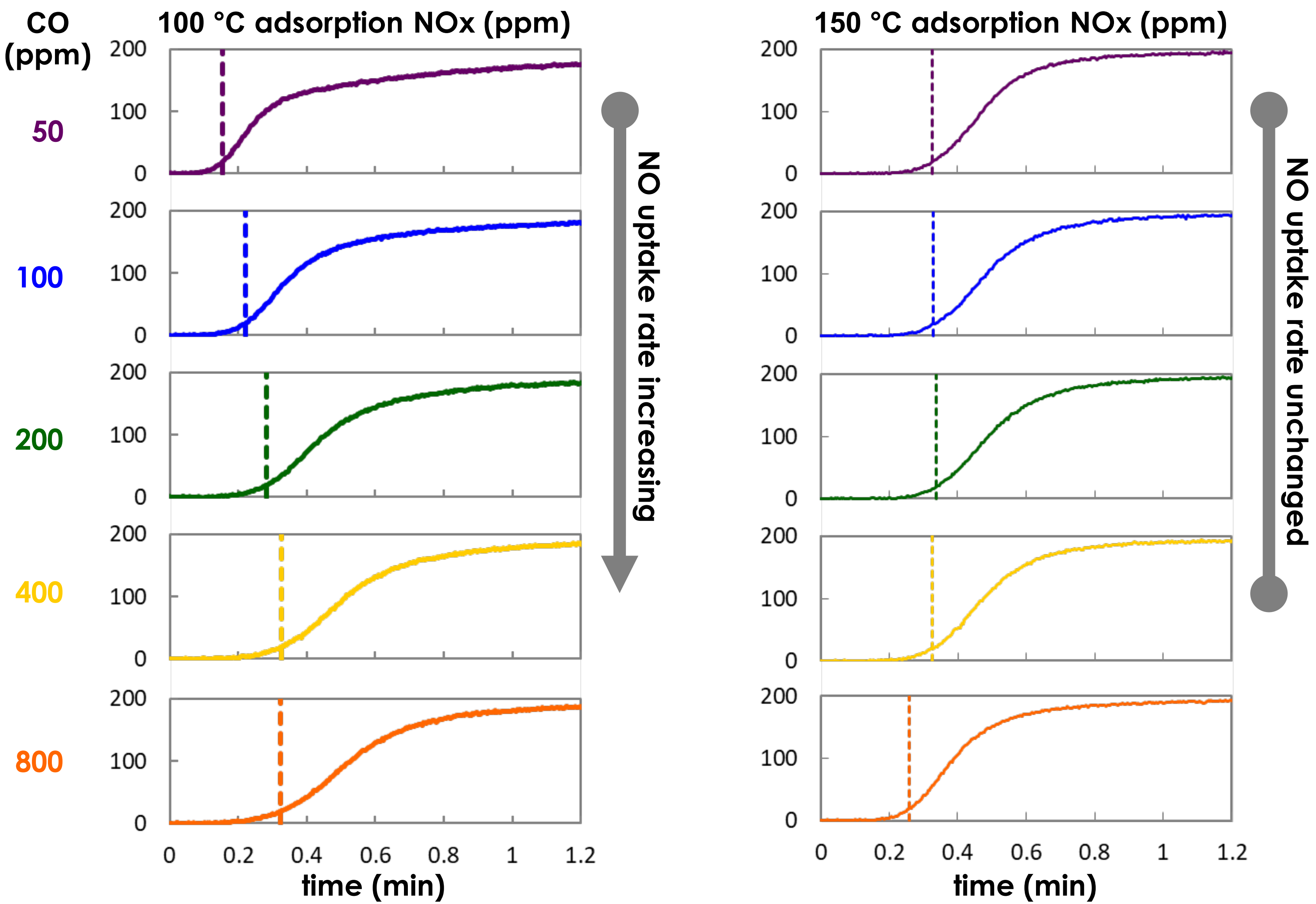
[1]*Consistent with Chen et al., Catal Lett 2016 146, 1706 (JM)*

Increasing H_2O decreases NO uptake[2] at 100 °C, but not at 150 °C



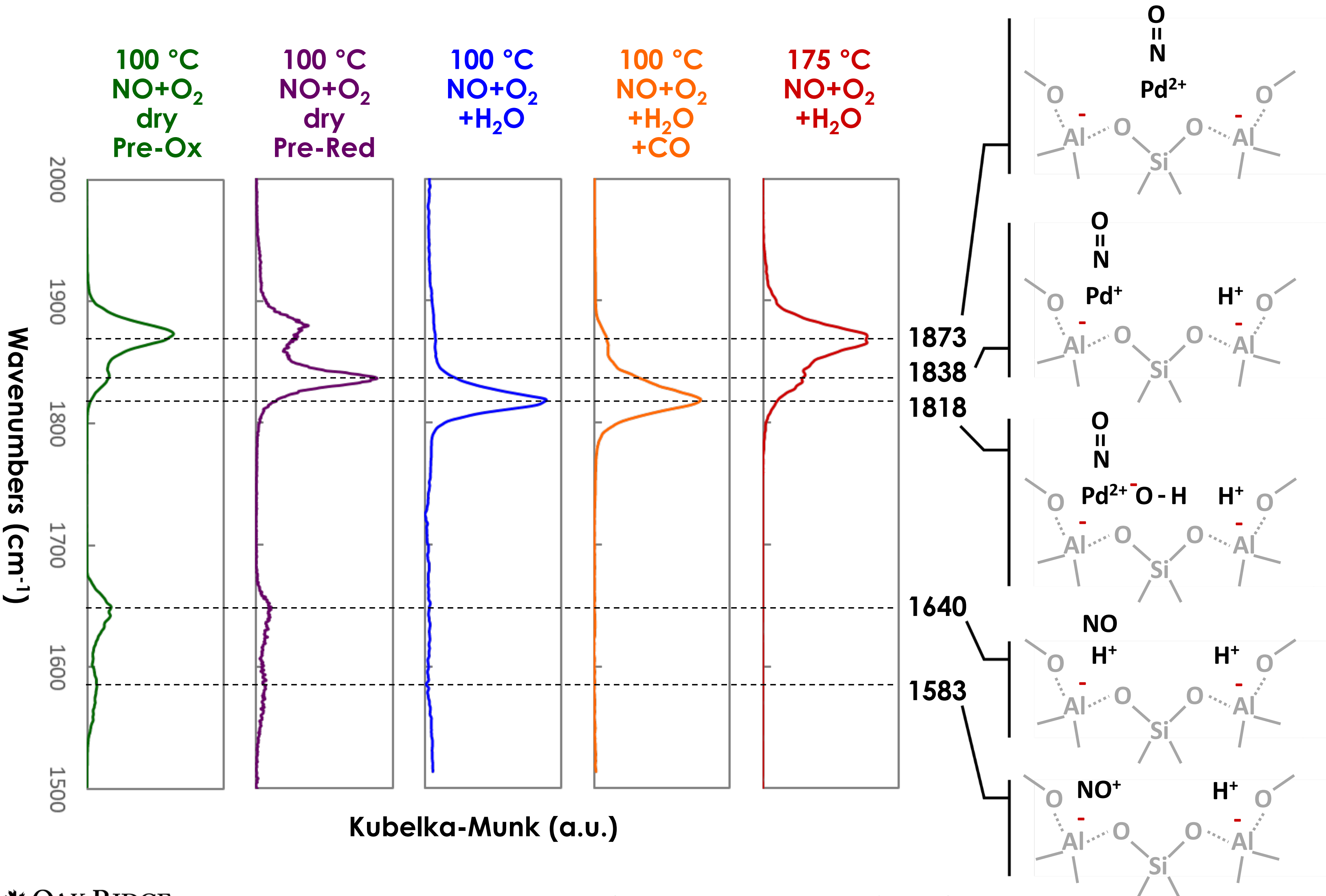
[2]Consistent with Zheng et al., J. Phys. Chem. C 2017, 121, 15793 (PNNL)

Increasing CO increases NO uptake[3] at 100 °C, but not at 150 °C

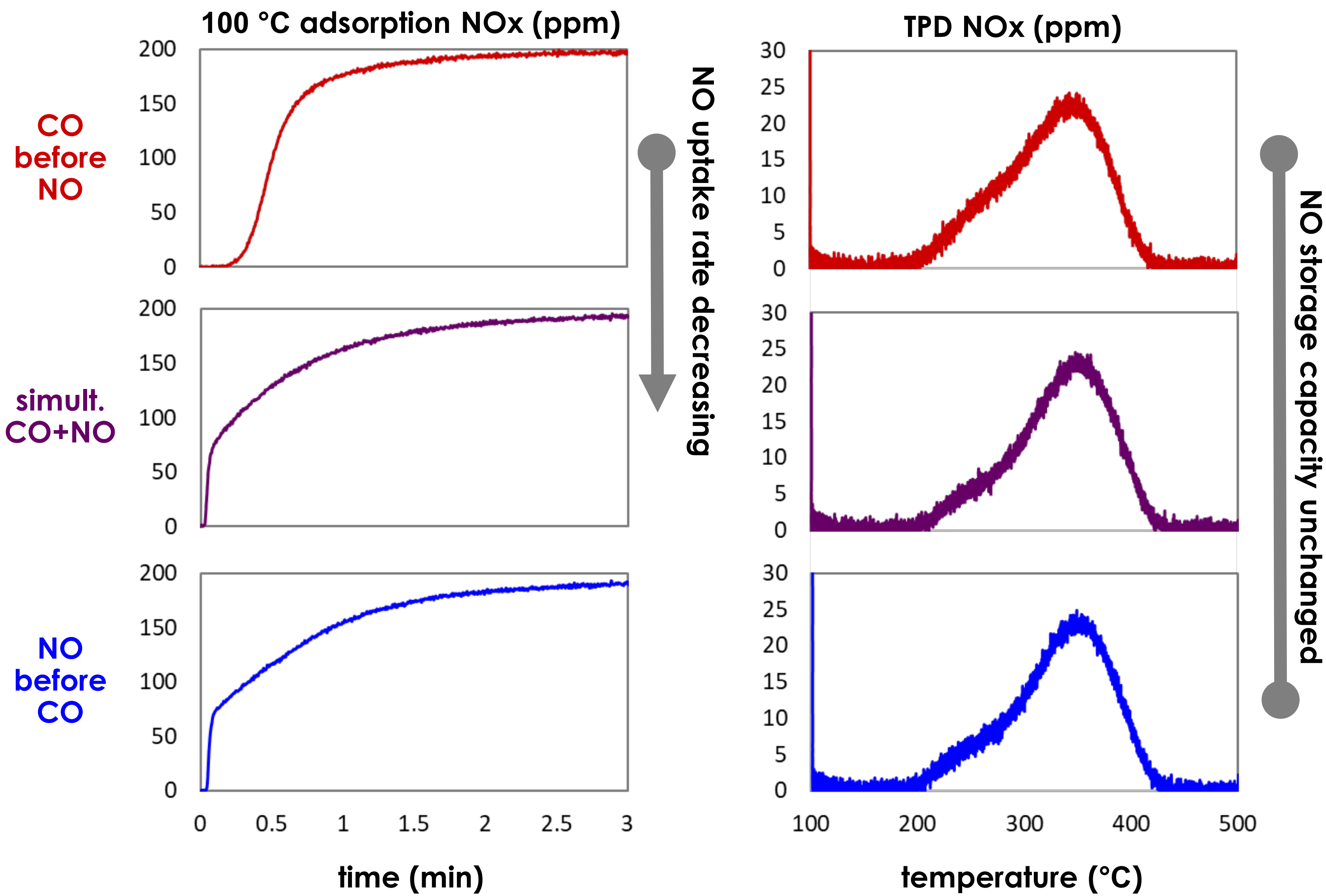


[3]*Consistent with Vu et al., Catal Lett 2017 147, 745 (UVA)*

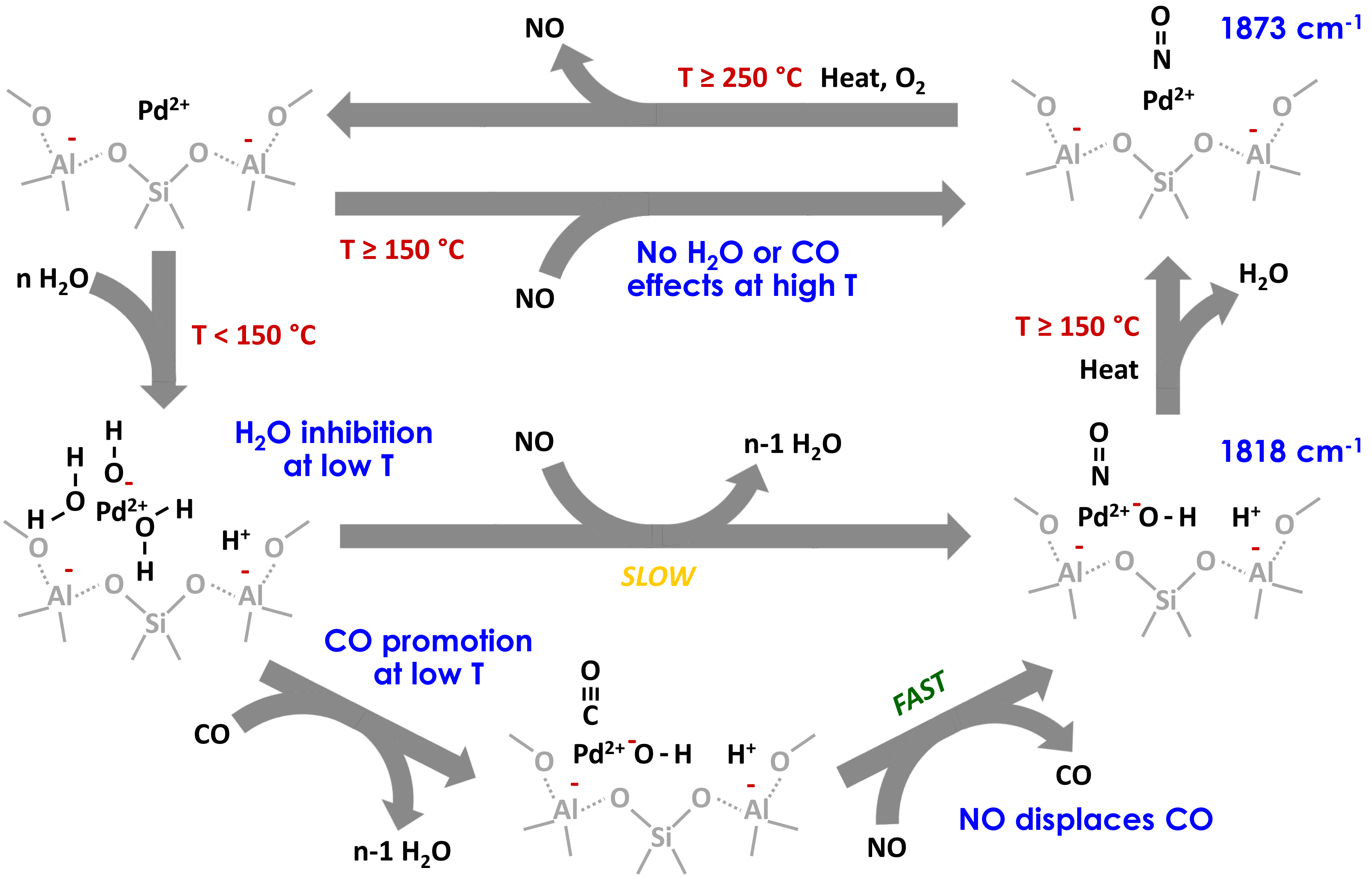
DRIFTS reveals three distinct NO/Pd adsorption configurations



CO increases the rate of NO uptake, but not the total equilibrium storage capacity



Proposed mechanism captures key gas composition & temperature effects, is consistent with DRIFTS observations, and provides a foundation for modeling efforts



Collaborations: 32 Industry, 23 Academic, 12 Natl. Labs/Govt.

CLEERS Technology Focus Group

Adv. Eng. Crosscut

ACEC TT

DOE VTO

LD OEMs:
FCA
Ford
GM

EPA
TARDEC

HD OEMs:
Caterpillar
Cummins
Daimler
Navistar
Paccar
Volvo

Suppliers:
BASF
Johnson-Matthey
Umicore
Corning
Delphi

CLEERS Industry Survey Recipients

Industry:
John Deere
Bosch
Tenneco
IAV
Emissol

Nat'l Labs:
ORNL
PNNL
ANL
LANL

Universities:
Chalmers Univ.
Michigan Tech. Univ.
Pennsylvania State Univ
Politecnico di Milano
Purdue Univ.
UCT Prague
Univ. of Houston
Univ. of Kentucky
Univ. of Notre Dame
Univ. of Michigan
Univ. of Virginia
Univ. of Wisconsin

CNH
Denso
Hyundai
Isuzu
NGK
Toyota

Aramco
AVL
CTS
Exothermia
Gamma
Faurecia
SPMC

CanmetEnergy
CPERI/CERTH
ECC Canada
KRICT
KIMM
NREL
SwRI

Binghamton Univ.
Karlsruhe Inst. of Tech.
Loughborough Univ.
Mass. Inst. of Tech.
Queens Univ. Belfast
Seoul National Univ.

SUNY at Buffalo
Univ. of Connecticut
Univ. of Mass. Amherst
Univ. of New Mexico
Univ. of Tennessee

CLEERS Participants

Responses to Comments from Reviewers

Reviewer Comments:	Responses:
• *"…would like to see more active interaction and engagement with catalyst suppliers"*	• Johnson Matthey provided PNA and HC trap materials • We share our plans and results with JM to get feedback
• *"The effects of S will be a ripe area for study as well, as well as the ability to desulfate the catalyst."*	• UVA will investigate sulfur effects on PNAs under our subcontract
• *"…there is perhaps too much focus on aftertreatment technologies (e.g., SCR) for diesel and other lean-burn engines. The reviewer suggested that it might be appropriate to look beyond conventional ICE's, such as hybrids…"*	• ORNL's CLEERS HC trap work is aimed at gasoline applications, including hybrids • If a promising PNA material for stoichiometric applications is developed, we will include it in our investigations
• *"…while CLEERS did a good job integrating properly modern gasoline engine developments in its focal discussions, it has been slow in directing sufficient focus from lean NOx trap to SCR to accommodate the HD diesel industry needs and trends"*	• Began working on SCR durability and modeling with PNNL in 2011 • Focused almost exclusively on SCR NH_3 storage and aging impacts 2014-2017 • Initiated low T trap work, including PNAs for HD diesel, in 2017

Remaining Challenges & Barriers/Future Work

Remaining Challenges:	**Future Work:** *(subject to change based on funding)*
• Ongoing need for coordination & collaboration in developing simulation tools for next generation emissions control devices	• Continue coordinating CLEERS activities: workshops, teleconferences, website, surveys
• Low exhaust temperatures from higher efficiency engines and advanced combustion modes. • 90% conversion of NOx and HCs at 150 °C	• Passive NOx Adsorbers: - Finalize and publish NO adsorption/ desorption mechanisms - Determine if other PNA materials follow the same mechanisms - Evaluate effects of sulfur exposure - Develop PNA modeling strategies • Hydrocarbon traps: - Measure adsorption isotherms for single HCs (ethanol, toluene, iso-octane, decane…) - Develop modeling strategies for HC adsorption/desorption

Summary

- **Relevance**
  - CLEERS supports the development of simulation tools for the design, optimization, and control of next generation advanced combustion engine/aftertreatment systems that maximize efficiency while still meeting emissions standards
- **Approach**
  - Promote sharing of precompetitive information among the emissions control community through workshops, teleconferences, website, and surveys
  - Develop modeling strategies, reaction mechanisms, parameter estimates, experimental protocols, and data sets to support development of aftertreatment simulation tools, with a particular focus on catalysts for low temperature exhaust
- **Technical Accomplishments**
  - Maintained high levels of participation in CLEERS activities
  - Conducted flow reactor and DRIFTS measurements of gas composition impacts on NO uptake on a PNA catalyst; developed a conceptual PNA model
- **Collaborations**
  - University of Virginia, Johnson Matthey, PNNL
  - Advanced Engine Crosscut Team, U.S.DRIVE ACEC Tech Team, CLEERS Participants
- **Future Work** *(subject to change based on funding levels)*
  - Continue coordination of CLEERS activities
  - Measure & model adsorption/desorption phenomena on PNAs and HC Traps

Technical Back-Up Slides

CLEERS is a team effort involving contributions from many people and organizations