

Advanced Water Gas Shift Membrane Reactor (DE-FC26-05NT42453)

T. H. Vanderspurt¹, S. C. Emerson¹, Z. Dardas¹, S. Opalka¹,
R. Radhakrishnan¹, S. Seiser¹, S. Tulyani¹, H. Wen¹, &
R. Willigan¹, W. Huang², T. B. Flanagan³, D. Wang³

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- 1) United Technologies Research Center, East Hartford, CT
- 2) QuesTek Innovations, Evanston, IL
- 3) Metal Hydride Technologies Inc., Burlington, VT

Project ID: PDP 26

Overview

Timeline

- Start – July 2005
- End – June 2007
- 46% Complete

Budget

- Total Project Funding
 - DOE share - \$849k
 - Contractor share - \$212k
- Funding Received in FY05
 - \$305k
- Funding for FY06
 - \$308k

Barriers

- Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan
 - Section 3.1.4.2.3: Separations and Other Cross-Cutting Hydrogen Production Barriers (DOE Office of Energy Efficiency and Renewable Energy)
 - M. Impurities
- Hydrogen from Coal – Research, Development, and Demonstration Plan
 - Section 5.1.5 Technical Barriers – Central Production Pathway (DOE Office of Fossil Energy)
 - D. Impurity Intolerance/Catalyst Durability
 - I. Poisoning of Catalytic Surfaces
 - Q. Impurities in Hydrogen from Coal

Partners

- QuesTek Innovations LLC
- Metal Hydride Technologies

Objectives

Overall

- Identify through Atomistic and Thermodynamic modeling a suitable Pd-Cu tri-metallic alloy membrane with high stability and commercially relevant hydrogen permeation in the presence of carbon monoxide and trace amounts of sulfur.
- Identify and synthesize a Water Gas Shift (WGS) catalyst with a high operating life that is sulfur and chlorine tolerant at low concentrations (0.004 atm Partial Pressure) of these impurities.

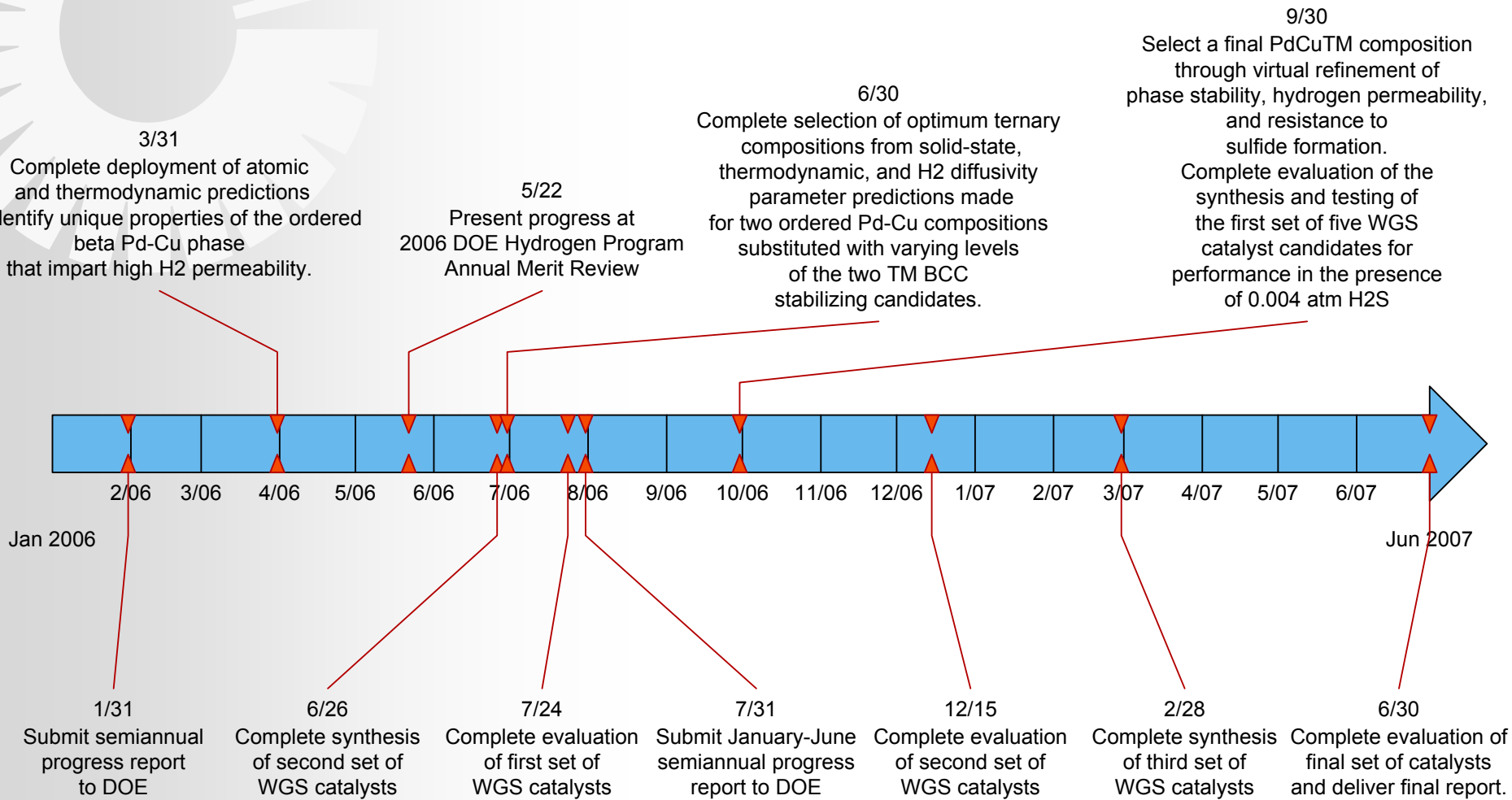
FY2006

- (Oct-Dec 2005) Complete screening and down-select from six to two Transition Metal (TM) substituents for PdCuTM alloy candidates demonstrating best potential to enhance stability of the ordered, beta (BCC) PdCu phase over an extended alloy composition and temperature range.
- (Jan-Mar 2006) Complete deployment of atomic and thermodynamic predictions to identify the unique properties of the ordered beta (BCC) Pd-Cu phase that impart high H₂ permeability.
- (Apr-Jun 2006) Complete selection of optimum ternary compositions from solid-state, thermodynamic, and H₂ diffusivity parameter predictions made for two ordered Pd-Cu compositions substituted with varying levels of the two TM BCC stabilizing candidates.
- (Jul-Sep 2006) Select a final PdCuTM composition through virtual refinement of phase stability, hydrogen permeability, and resistance to sulfide formation. Complete evaluation of the synthesis and testing of the first set of five WGS catalyst candidates for performance in the presence of 0.004 atm H₂S.

Combine Hydrogen Separation with ~43 Atm. Water Gas Shift ($\text{H}_2\text{O} + \text{CO} \rightleftharpoons \text{H}_2 + \text{CO}_2$) in Presence of H_2S & COS

- Some Pd-Cu alloys reportedly have sulfur tolerance and the BCC Pd-Cu phase has high H permeance but lower thermal stability and questionable chemical stability in the presence of Sulfur and CO_x than the FCC phase.
- **Approach:** Use VASP atomistic modeling and thermodynamic parameter estimation to predict higher stability BCC Pd-Cu based trimetallic alloys with commercial relevant permeance.
- Pt-Re/Doped Ceria-Zirconia and Pt-Re/Titania based catalysts have been reported to have acceptable volumetric Water Gas Shift Activity at ~ 1 Atm and ~ 2 ppmv H_2S with natural gas or diesel reformat.
- **Approach:** Combine: 1) Prepare high surface area, low mass transfer resistance, very high dispersion Pt base mixed metal cluster catalysts on doped nano-engineered oxides. 2) Chose dopants that are likely to increase sulfur tolerance using VASP atomistic modeling. 3) Validate modeling approach through kinetic evaluation with and without sulfur and after aging in 0.004 atm H_2S reformat. Down select to final composition.

Plan and Time Line



Critical Assumptions and Issues

Assumptions

- Atomistic & Thermodynamic Modeling will be a reliable guide to new Sulfur Tolerant, thermally stable membrane with commercial relevant hydrogen permeance.
- High H_2O to H_2S Partial Pressure will mitigate support sulfidation and oxy-sulfidation
- Dopants can mitigate oxide over-reduction at high H_2 and CO partial pressures
 - Preventing over reduction should prevent excessive surface carbonate formation
- In the Pt-Re/CeZrOx case, the Gorte mechanism is the dominant WGS route

Issues

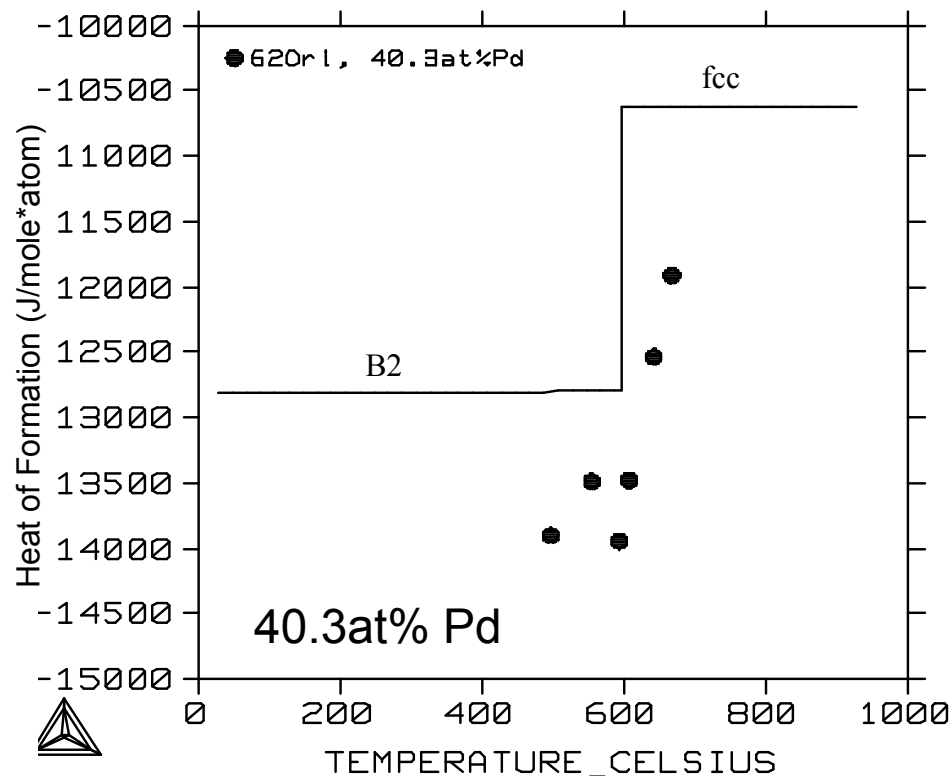
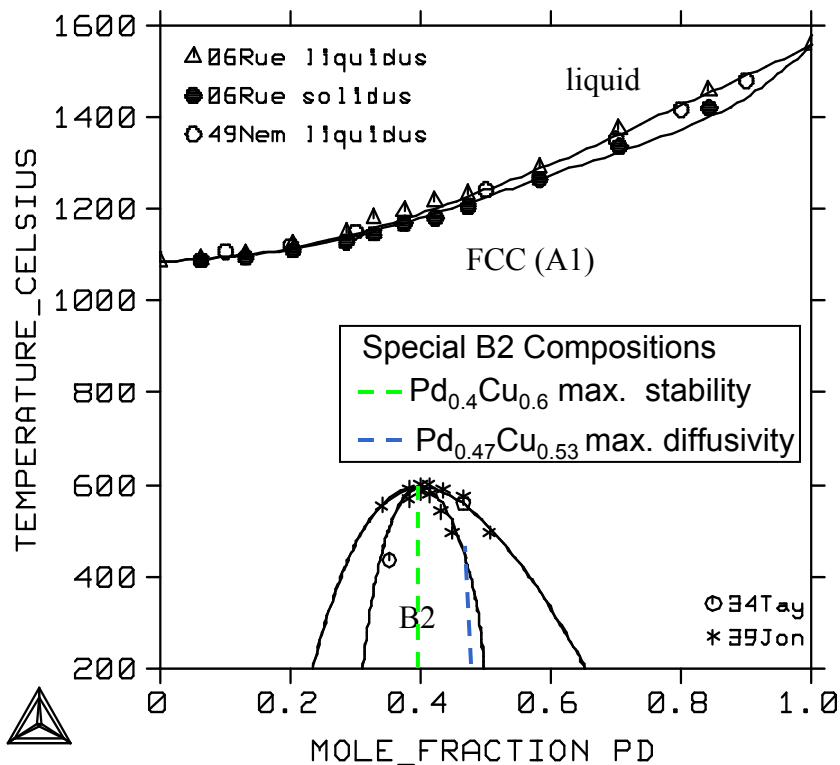
- Achieving stable, equal flow operation across all 5 reactors under target conditions at ~ 43 atm total pressure with high steam to CO ratio proved to be very difficult.
 - Initial calibrated orifice design unreliable
 - New larger diameter steam generator and other modifications being implemented
 - 2nd set of catalysts will be tested under target conditions.

Outline of Technical Progress

- Atomistic and Thermodynamic Modeling of potential trimetallic BCC phase PdCuTm alloys
 - Down selection of two leading candidates
 - Benchmarking B2 phase PdCuH system
- Atomistic modeling of potential dopants for the TiO₂ based catalyst system.
- Identification and some physical characterization of first set of 5 Pt-Re Oxide catalysts
- Initial sulfur free catalyst performance results

New Thermodynamic Model for Pd-Cu Binary System

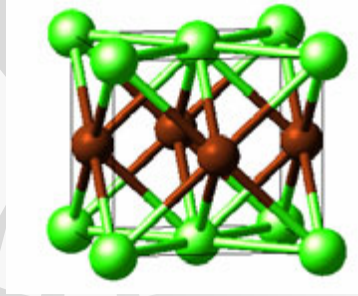
First step to a viable model for BCC phase trimetallic Pd-Cu-TM w & w-o H₂



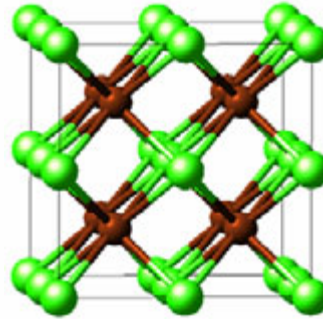
A complete Cu-Pd thermodynamic description including the ordered B2 phase.

Thermodynamic & First-Principles Modeling Comparison

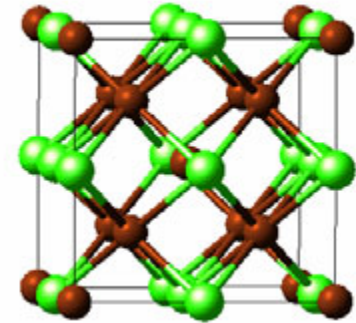
VASP minimized structures using PAW GGA PW hard potentials:



Pd_{0.5}Cu_{0.5} ordered FCC
a=3.805 Å

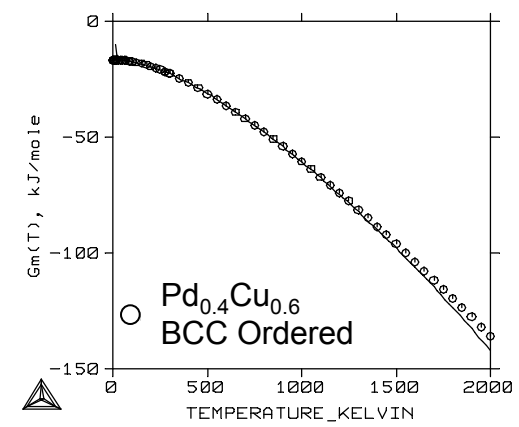
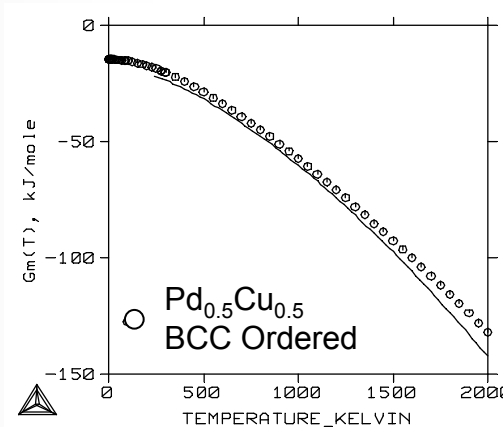
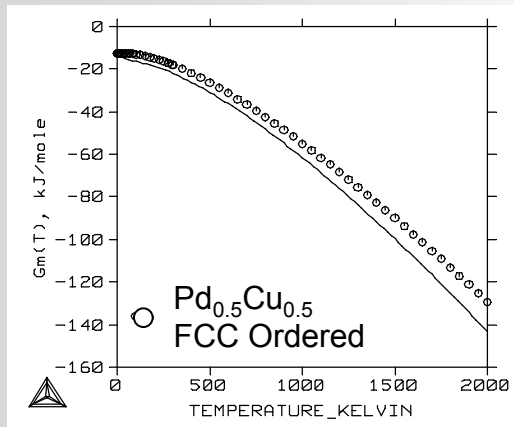


Pd_{0.5}Cu_{0.5} B2 2x2x2
a=3.013 Å



Pd_{0.4}Cu_{0.6} B2 2x2x2
a=2.982 Å

Comparison of MedeA Phonon direct method thermodynamic predictions (○) with thermodynamic modeling of experimental data (—):



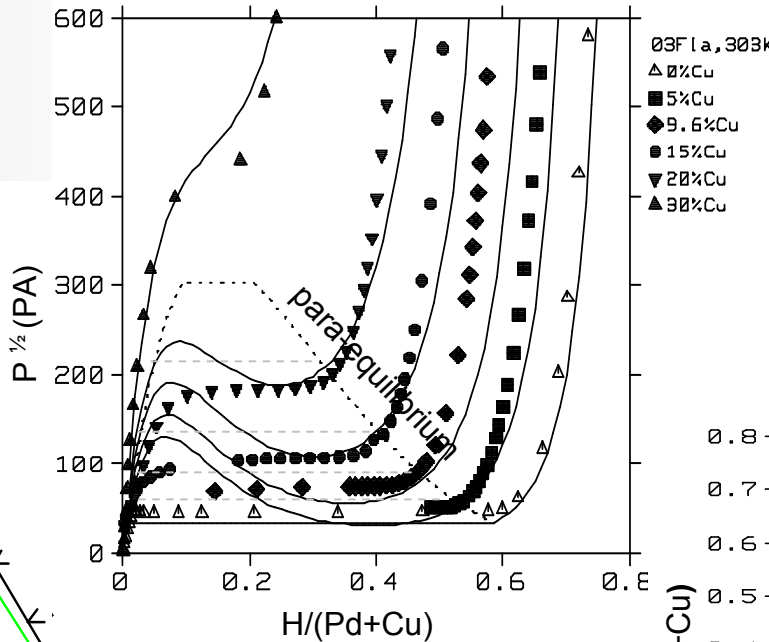
Excellent agreement serves to validate first-principles thermodynamic predictions. High stability of Pd_{0.4}Cu_{0.6} ordered B2 phase confirmed.



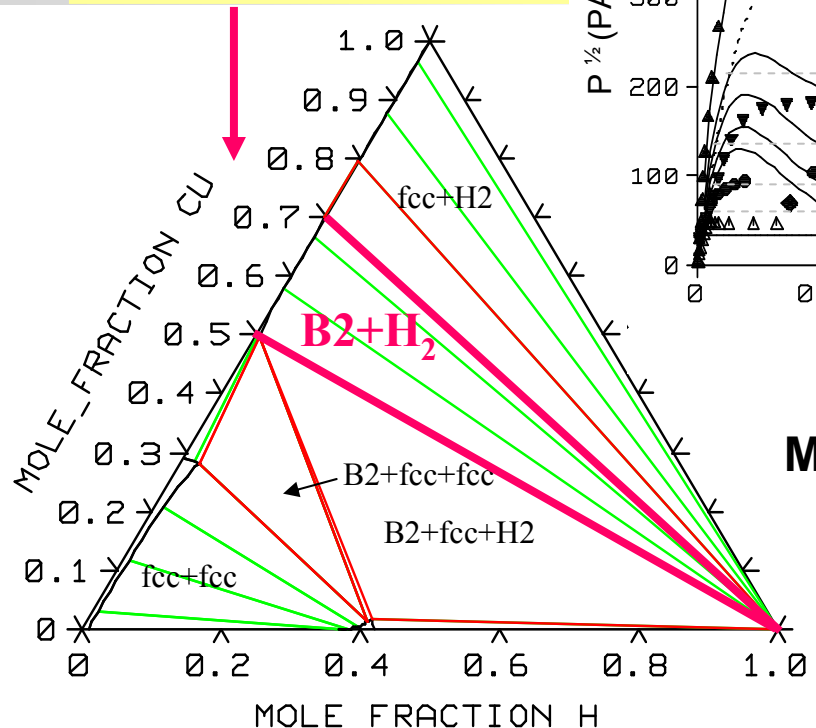
New H Solubility In PdCu B2 Phase Data Incorporated Into Thermodynamic Model

Thermodynamic Model

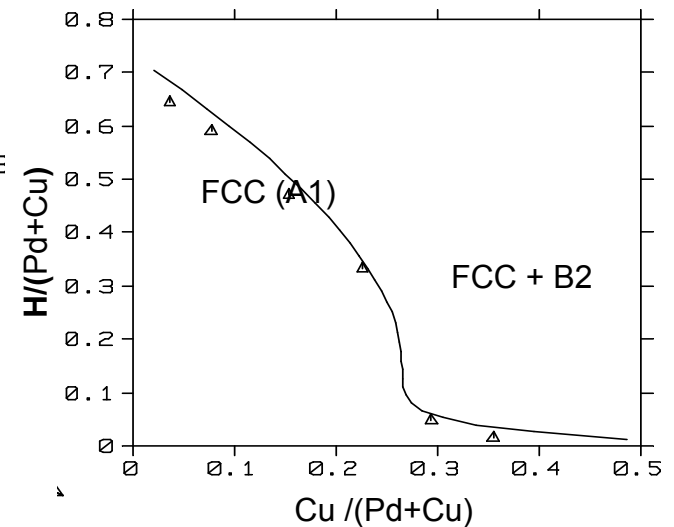
B2 Phase Pd-Cu composition narrows with increasing H content



Experimental Data



FCC-FCC Miscibility Gap



H Solubility in CuPd alloys

T= 298 K P=10⁵ Pa

Pd-Cu-H Section T= 303 K P=10⁵ Pa

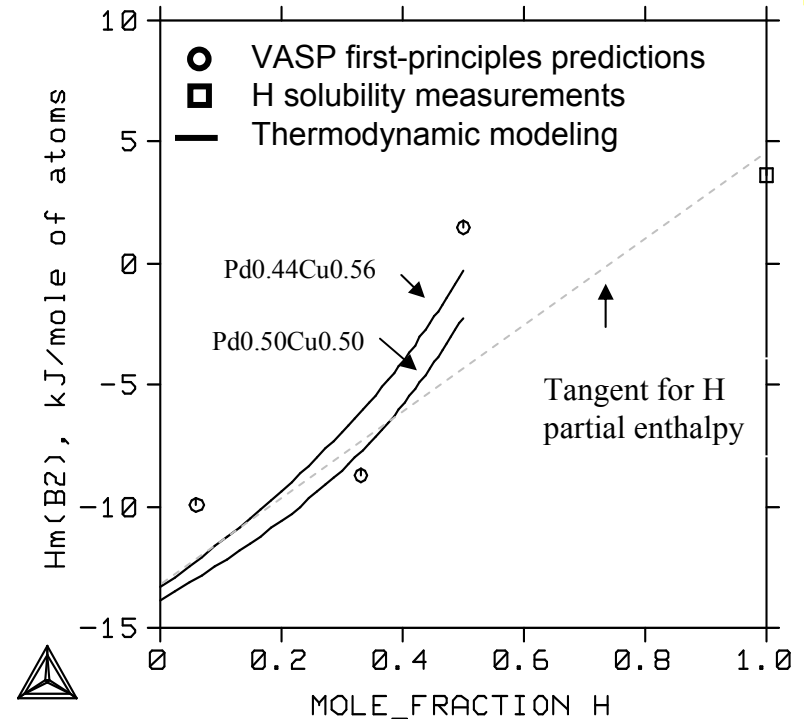
Combined First-Principles, Experimental, and Thermodynamic Investigations of H in PdCu B2

Observation & prediction agreement increases confidence in PdCuTm H work

0.06 Mole-Fraction H in Pd _{0.5} Cu _{0.5} Ordered B2		
Full Ground State Minimization		
H Interstitial Site	ΔV (cm ³ /MoleH)	$\Delta H_{\text{form elect}}$ (0K) (kJ/Mole*atom)
Alpha-Octahedral	0.12	-8.64
Beta-Octahedral	0.10	-9.28
Tetrahedral	0.12	-9.43

Diffusion Coefficient Comparison	D (m ² /s)
Phase / Source	at 57 C/ 330 K
BCC Pd _{0.50} Cu _{0.50} Prediction (UTRC)	2.20E-09
BCC Pd _{0.47} Cu _{0.53} Experiment (Völkl, 1978)	5.73E-09
FCC Pd _{0.47} Cu _{0.53} Experiment (Völkl, 1978)	1.80E-12

J. Völkl, G. Alefeld, in *Hydrogen in Metals*, Vol. I, G. Alefeld, J. Völkl, Eds., Berlin: Springer Verlag, (1978).



The enthalpy of formation at 298°K, relative to pure element at 298°K (fcc-Cu, fcc-Pd, gas-H₂). The calculated partial H(H) is 4.45 kJ/mole H, experimental 3.6 kJ.

H solubility and diffusivity parameters benchmarked in PdCu B2 system.



Transition Metal (TM) Substitution in Pd_{0.5}Cu_{0.5} B2

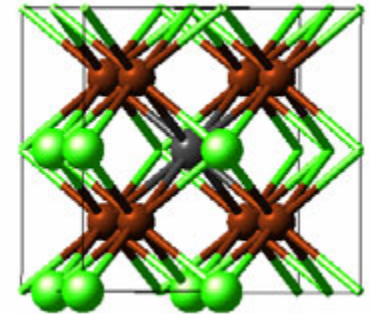
Composition	$\Delta H_{\text{sub elect}}(0 \text{ K})$ (kJ/mole*atom)	ΔVolume (Å ³ /atom)
Pd ₈ Cu ₈	-	-
Pd ₈ Cu ₇ (R4)	2.17	-0.01
Pd ₇ (T5)Cu ₈	0.84	0.14
Pd ₈ Cu ₇ (G5)	-7.12	0.42
Pd ₈ Cu ₇ (J5)	2.39	0.29
Pd ₈ Cu ₇ (G6)	-9.67	0.42
Pd ₈ Cu ₇ (J6)	1.64	0.29
Pd ₈ Cu ₇ (G4)	-4.17	0.10

VASP: PAW GGA PW hard potentials

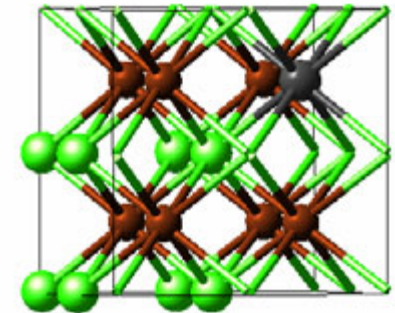
TM = R4, T5, G4, G5, G6

$$\Delta H_{\text{sub elect}}(0 \text{ K}) = E(0 \text{ K})_{\text{composition}} - (E(0 \text{ K})_{\text{Pd}_8\text{Cu}_8} + E(0\text{K})_{\text{TM}})$$

TM substituted in
Pd₈Cu₈ 2x2x2



Pd₇TMCu₈ TM substituted for **Pd**



Pd₈Cu₇TM TM substituted for **Cu**

Substitution of most TM more favorable on Cu sublattice. Some TM have both favorable, exothermic heats of substitution and increased volume.

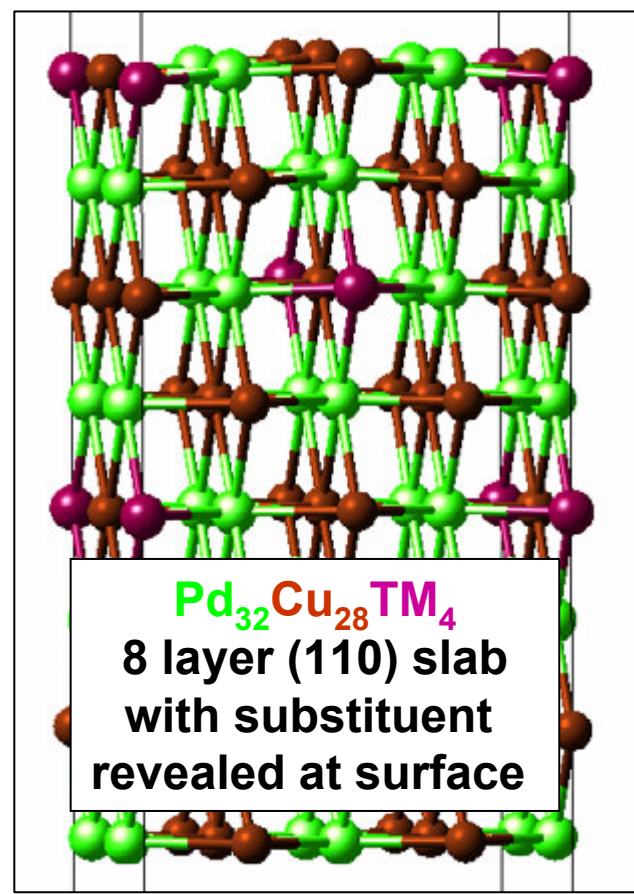
TM Substitution Influence on Pd_{0.5}Cu_{0.5} B2 (110) Slab

Sub-surface sites favored by most TM substituents

Composition 110 2x2x2 Slab	$\Delta H_{\text{form elect}}$ (0 K) (kJ/mole*atom)	Surface Energy J*/m ² (0 K)
Pd ₃₂ Cu ₃₂	3.85	1.37
Pd ₂₈ Cu ₃₂ (T5) ₄	4.81	1.37
Pd ₃₂ Cu ₂₈ (G5) ₄	-2.24	1.45
Pd ₃₂ Cu ₂₈ (G6) ₄	-4.59	1.47
Pd ₃₂ Cu ₂₈ (J6) ₄	6.67	1.47
Pd ₃₂ Cu ₂₈ (G4) ₄	0.55	1.45

VASP: PAW GGA PW hard potentials

$$\text{Surface Energy} = (E_{\text{slab}}(0 \text{ K}) - E_{\text{bulk}}(0 \text{ K})) / (2 * \text{surface area})$$



Most TM substituents increase surface energy, indicating a negative tendency for substituent surface segregation.

Down-selection of TM Alloying Agent for Pd_{0.5}Cu_{0.5} B2

Modeled Property	TM Substituent – G5	TM Substituent – G6	TM Substituent – J6
Alloy $\Delta H_{\text{substitution}}$	Very spontaneous	Very spontaneous	Slightly endothermic
Alloy ΔVolume	Significant	Significant	Somewhat significant
Alloy Surface Energy	High	High	Very High
TM Oxidation	Very High	Very High	High, may be reducible
TM Sulfidation	Very low	Very low	Low
Pd-TM Intermetallic	Yes	Yes	Possible
TM-H Hydrides	Yes	Yes	No
TM Cost	Low	10X higher	Low

Virtual down-selection criteria included substitution favorability, impact on structure, substituent reactivity, competing substituent phases, and cost.

VASP Calculations Show That Properly Doped TiO₂ System May Have Advantages Over Non-doped TiO₂ For H₂S Operation

High steam to H₂S ratio may be necessary to prevent oxide sulfidation

System	H ₂ S-Pt eV	OC-Pt eV	OC-Oxide eV	H ₂ S- Oxide eV
Pt/TiO ₂ Anatase (101)	-0.76	-1.67		
Pt/Ti _(1-x) J6 _x O ₂	-0.40	-0.97		
PtCe _{0.5} Zr _{0.42} J6 _{0.08} O ₂	-2.04	-1.74		
TiO ₂ Anatase (101)			-0.32	-1.93
Ti _(1-x) J6 _x O ₂ Surface			-0.85	-2.17
Ce _{0.5} Zr _{0.42} J6 _{0.08} O ₂ Surface			-0.63	-2.14

- H₂O vs oxide surface and CO, H₂O and H₂S versus subsurface dopants underway

WGS Catalyst Development - Oxide Characterization

4 of 5 Catalysts satisfy requirements for desired state

Surface Area / Pore Volume Information

<u>Target Material</u>	<u>Surface Area (m²/g)</u>	<u>Pore Volume (cm³/g)</u>	<u>Pore Diameter (Å)</u>
1. Ce _{0.53} Zr _{0.38} J6 _{0.1} O ₂	216	0.28	53
2. TiO ₂	238	0.53	91
3. Ti _{0.8} Ce _{0.2} O ₂	290	0.64	88
4. Ce _{0.333} Zr _{0.333} E4 _{0.333} O ₂	246	0.39	63
5. Ce _{0.3} Zr _{0.3} E4 _{0.3} J6 _{0.1} O ₂	244	0.44	72

Structural Information

<u>Target Material</u>	<u>Desired State</u>	<u>Phase (by XRD)</u>	<u>Crystal Size</u>
1. Ce _{0.53} Zr _{0.38} J6 _{0.1} O ₂	Cubic CeO ₂ , no separate J6Ox phase	64% cub /36% tetr, no J6Ox	2.5 nm
2. TiO ₂	Anatase (100%)	85% anatase, 15% brookite	6.2 / 1.7 nm
3. Ti _{0.8} Ce _{0.2} O ₂	Single doped phase	Multi-Phase Separation (TiO ₂ , CeO ₂ , Ce ₂ TiO ₅ , Ce ₂ TiO ₇)	
4. Ce _{0.333} Zr _{0.333} E4 _{0.333} O ₂	Cubic CeZrO ₂ , no separate E4Ox phase	70% cub/ 21% tetr, no anatase	2.4 nm
5. Ce _{0.3} Zr _{0.3} E4 _{0.3} J6 _{0.1} O ₂	Cubic CeZrO ₂ , no separate E4Ox or J6Ox phase	100% cubic	2.0 nm

WGS Catalyst Development - Platinum / Rhenium Loading

Results

CATALYST	COMPOSITION (by synthesis)	COMPOSITION (by ICP analysis)	DESIRED Pt wt%	Achieved Pt wt%	Re wt% loaded
ST WGS-01	$\text{Ce}_{0.53}\text{Zr}_{0.38}\text{J6}_{0.1}\text{O}_2$	$\text{Ce}_{0.54}\text{Zr}_{0.35}\text{J6}_{0.11}\text{O}_2$	2.0	2.09	1.045
ST WGS-02	TiO_2	TiO_2	2.0	0.60	0.30
ST WGS-05	$\text{Ti}_{0.8}\text{Ce}_{0.2}\text{O}_2$	$\text{Ti}_{0.88}\text{Ce}_{0.12}\text{O}_2$	2.0	2.11	1.055
ST WGS-06	$\text{Ce}_{0.333}\text{Zr}_{0.333}\text{E4}_{0.333}\text{O}_2$	$\text{Ce}_{0.36}\text{Zr}_{0.32}\text{E4}_{0.33}\text{O}_2$	2.0	1.97	0.985
ST WGS-07	$\text{Ce}_{0.3}\text{Zr}_{0.3}\text{E4}_{0.3}\text{J6}_{0.1}\text{O}_2$	$\text{Ce}_{0.32}\text{Zr}_{0.28}\text{E4}_{0.31}\text{J6}_{0.09}\text{O}_2$	2.0	1.74	0.87

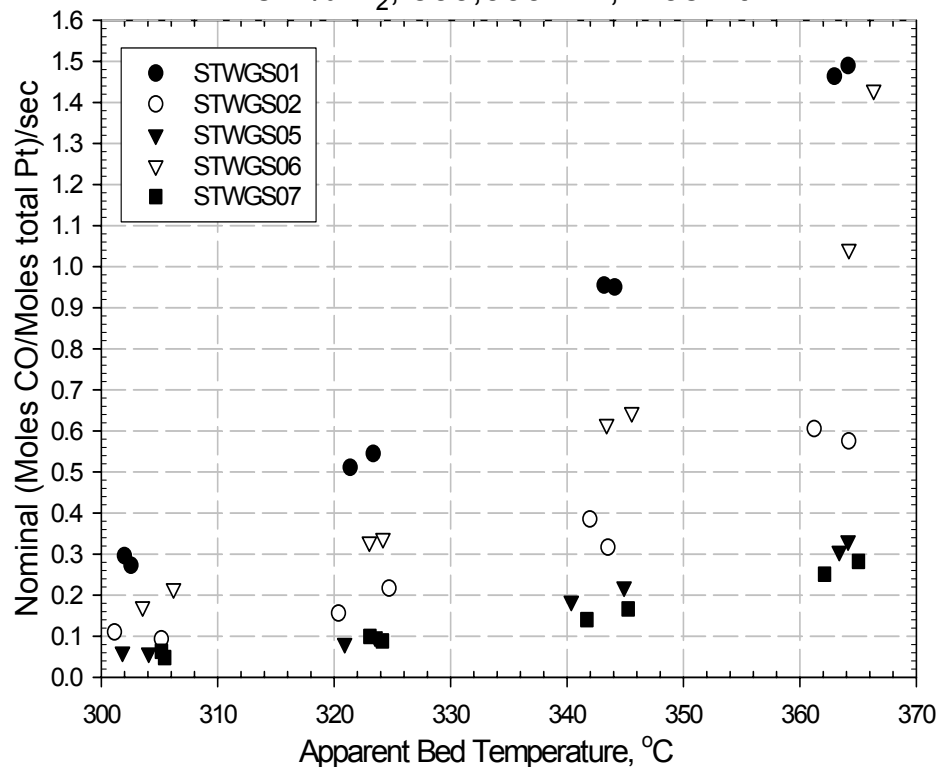
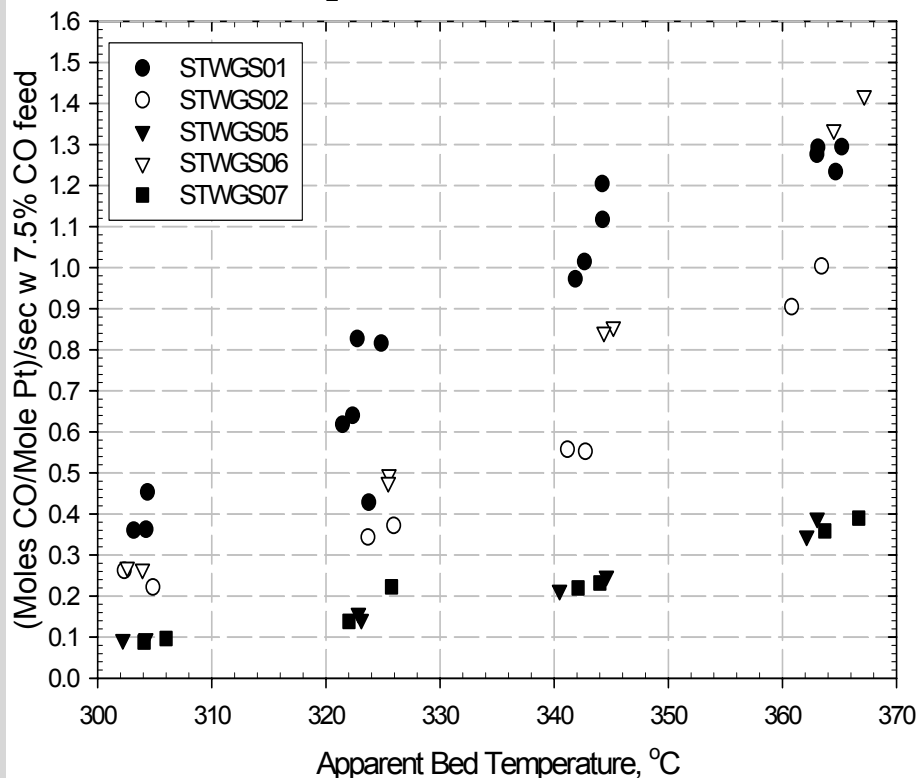
Two Catalyst Families Down Selected for Next Phase

Subject to H₂S Aging Study Currently Underway

- Ceria Based: Ce_{0.50}Zr_{0.40}J6_{0.10}O_x & Ce_{0.33}Zr_{0.33}E4_{0.33}O_x
- Titania Based: TiO₂ (Ti_{0.9}J6_{0.1}O₂ and Ti_(1-x)Dp_xO₂)

7.5% CO, 31.6% H₂O, 7.9% CO₂, 6.4% H₂,
46.6% N₂, 300,000 hr⁻¹, 1.05 Atm

14.0% CO, 31.0% H₂O, 14.9% CO₂, 12.0% H₂,
28.1% N₂, 300,000 hr⁻¹, 1.05 Atm

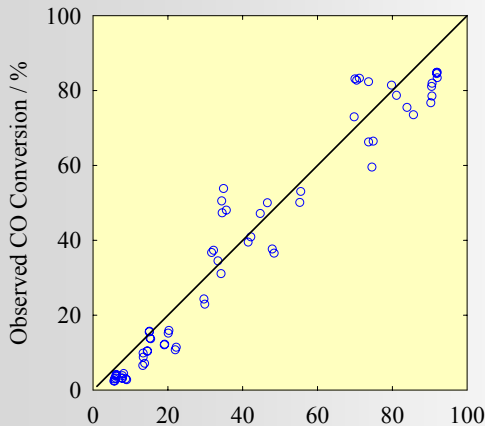


Early Kinetics Suggest Key Mechanistic Differences

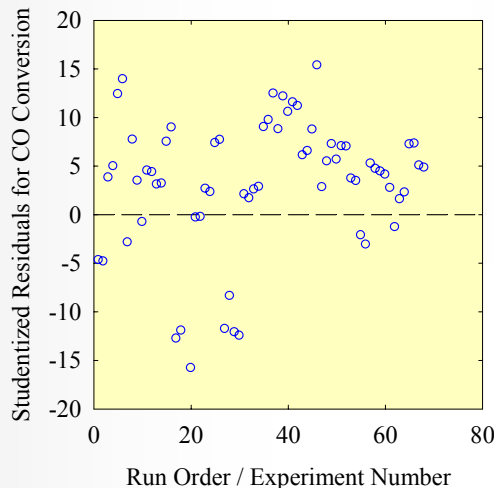
Multiple site or Gorte type mechanism evident in Pt-Re/Ce_{0.53}Zr_{0.38}J6_{0.1}O₂ while Pt-Re/ TiO₂ seems dominated by metal site mechanism.

Catalyst	Composition (by synthesis)	n _{CO}	n _{H₂O}	n _{CO₂}	n _{H₂}	E / kJ.mol ⁻¹
STWGS-01	Ce _{0.53} Zr _{0.38} J6 _{0.1} O ₂	0.32	1.0	0.85	0.87	51.4±0.1
STWGS-02	TiO ₂	-0.22	0.85	0.57	0.28	75.5±6.8
STWGS-05	Ti _{0.8} Ce _{0.2} O ₂	1.0	1.0	0.70	0.81	81.5±8.4
STWGS-06	Ce _{0.333} Zr _{0.333} E4 _{0.333} O ₂	0.70	1.0	0.73	1.0	72.4±9.6
STWGS-07	Ce _{0.3} Zr _{0.3} E4 _{0.3} J6 _{0.1} O ₂	1.0	1.0	0.72	0.78	70.2±7.0

Parity Plot for STWGS01



Residuals Plot for STWGS01



$$r_{WGS} = k P_{CO}^{n_{CO}} P_{H_2O}^{n_{H_2O}} P_{CO_2}^{n_{CO_2}} P_{H_2}^{n_{H_2}} \times (1 - \beta)$$

$$\beta = \frac{P_{CO_2} P_{H_2}}{P_{CO} P_{H_2O} K_{eq}}$$

- Additional kinetics, sulfur and aging experiments planned

Future Work

- (Apr-Jun '06) Complete selection of optimum ternary compositions from solid-state, thermodynamic, and H₂ diffusivity parameter predictions made for two ordered Pd-Cu compositions substituted with varying levels of the two TM BCC stabilizing candidates.
- (Jul-Sep '06) Select a final PdCuTM composition through virtual refinement of phase stability, hydrogen permeability, and resistance to sulfide formation. Complete evaluation of the first set of five WGS catalyst candidates for performance in the presence of 0.004 atm H₂S. Identify through a combination of modeling and kinetic analysis and the prepare the next set of 5 WGS Catalyst candidates
- (Oct-Dec '06) Determine sulfur free kinetics of 2nd set of 5 catalysts.
- (Jan-Mar '07) Complete evaluation of 2nd set of 5 catalysts and complete catalyst atomistic modeling and synthesize final set of catalysts.
- (Apr-Jun '07) Complete evaluation of final set of catalysts and deliver final report.

Advanced Membrane Reactor Water Gas Shift Summary

Relevance Lower cost high purity H₂ production from precleaned coal gas:
Eliminates need for: 1) complete sulfur scrubbing, 2) separate H₂ extraction/purification train and retentate gas is >90% CO₂ on a dry basis.

Approach

- Atomistic and thermodynamic modeling to design high stability BCC Pd-Cu based trimetallic alloy with commercial relevant permeance.
- Design synthesize and test catalyst tailored to needs of AMR

Accomplishments

- Two “stabilized” BCC alloys Pd_{0.5}Cu_(0.5-x)G5_x and Pd_{0.5}Cu_(0.5-x)J6_x down selected.
- Dopants that could potentially reduce H₂S impact on Pt based WGS activity identified.

Issues

- Mechanical difficulties have delayed high pressure and sulfur testing, but identification of next set of 5 catalysts still expected in July

Responses to Previous Year Reviewers' Comments

- Project underway less than 1 year, no reviewers' comments form last year

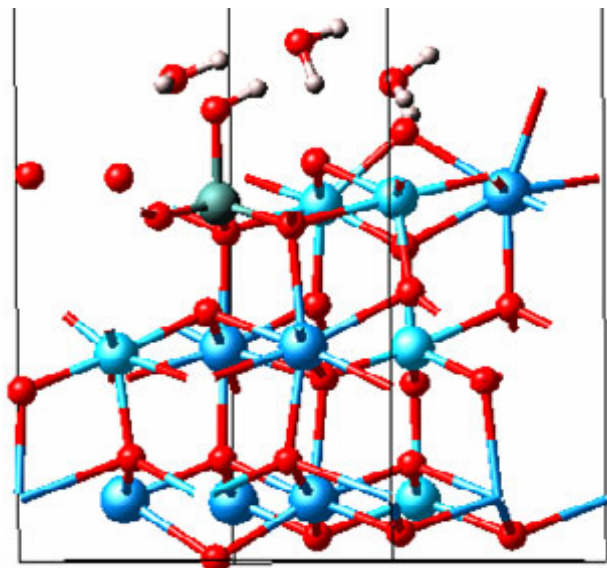
Publications and Presentations

- S. M. Opalka, T. H. Vanderspurt, S. C. Emerson, D. A. Mosher, Y. She, X. Tang, and D. L. Anton, "Theoretical Contributions Towards the Development of Storage Media and Related Materials for Hydrogen Processing", invited presentation, 2006 TMS Annual Meeting, San Antonio, Texas, March 13-16, 2006.
- S. M. Opalka, Y. She, W. Huang, D. Wang, T. B. Flanagan, S. C. Emerson, and T. H. Vanderspurt, "Hydrogen interactions with the ordered BCC PdCu alloy," invited presentation to be given at MH2006 International Symposium on Metal-Hydrogen Systems, Lahaina, HI, October 1-6, 2006.

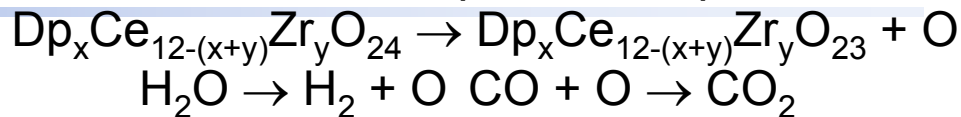
BACKUP

- Slides reflect either work from past efforts or details from present effort

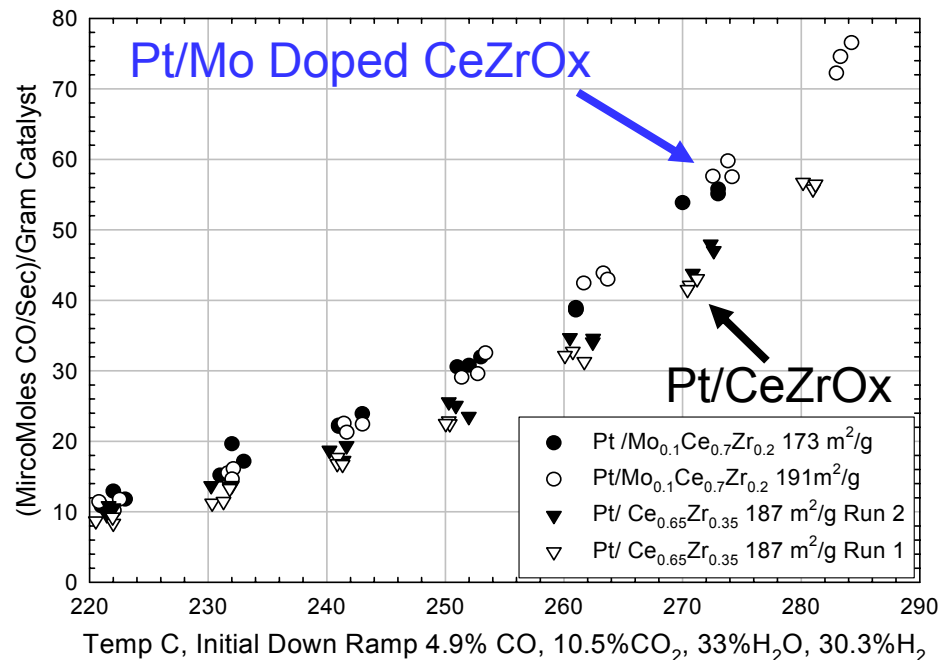
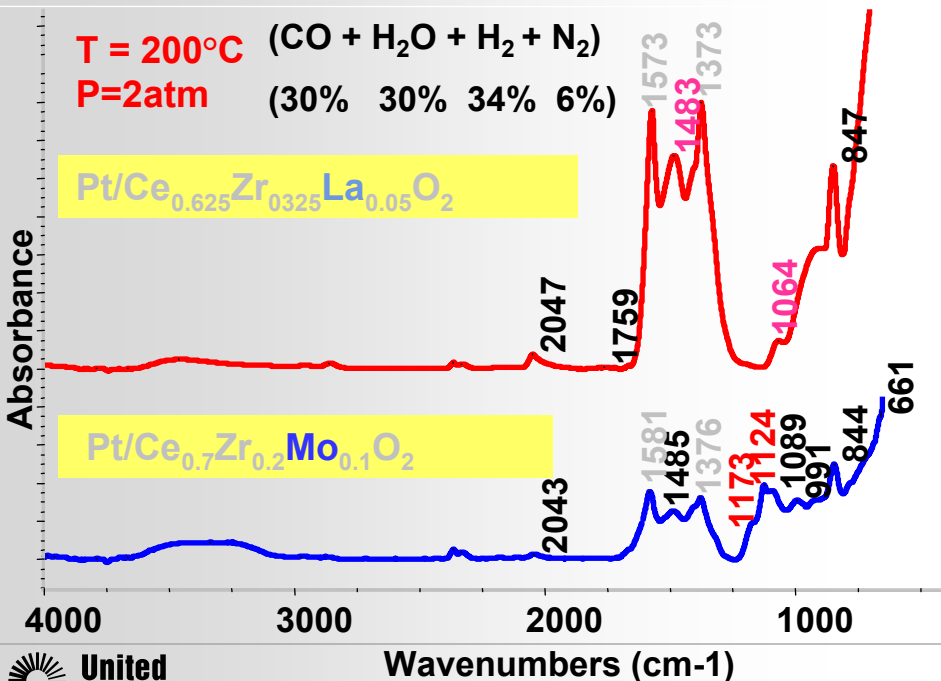
VASP Modeling Insights Led To Better Catalysts



Calculated Coupled Enthalpies



Oxide Slab	kJ/Mole	kJ/Mole
Ce ₁₂ O ₂₄	+154.5	-222.4
Ce ₇ Zr ₅ O ₂₄	+154.5	-222.1
TaCe ₆ Zr ₅ O ₂₄	-77.2	9.6
MoCe ₆ Zr ₅ O ₂₄	-48.3	-19.3

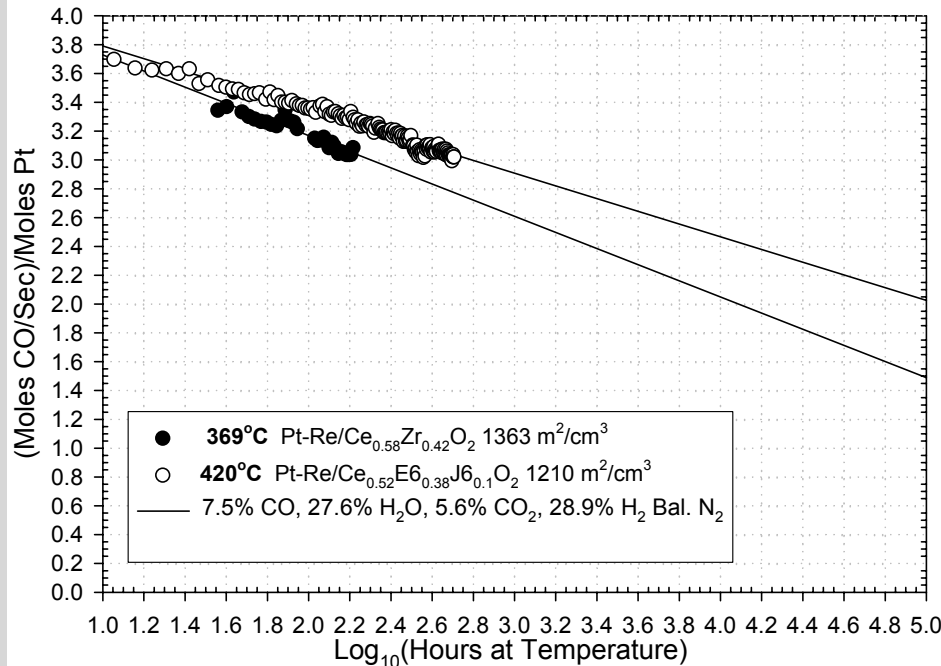


Higher Activity Catalyst w Similar Pt & SA

Doping Has Increased Catalyst Thermal Robustness

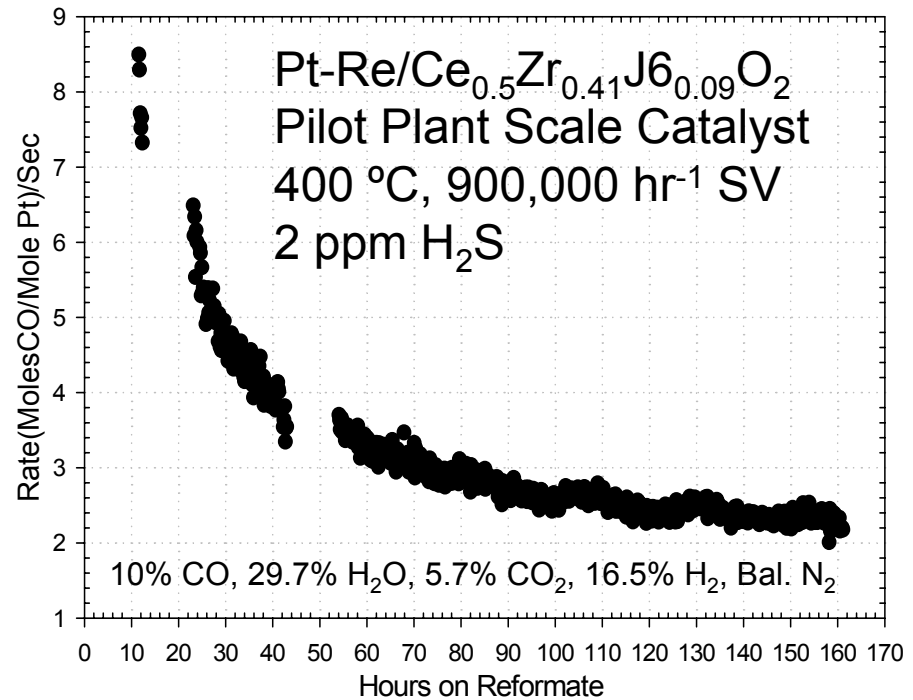
- $\text{Ce}_{0.52}\text{Er}_{0.38}\text{Jr}_{0.1}\text{O}_2$ retains estimated 65% of 100 hr lined out activity after 40,000 hr at 420°C w/o S

- $\text{Ce}_{0.58}\text{Zr}_{0.42}\text{O}_2$ catalyst retains estimated 54% of 100 hr lined out activity after 40,000 hr at 369°C w/o S

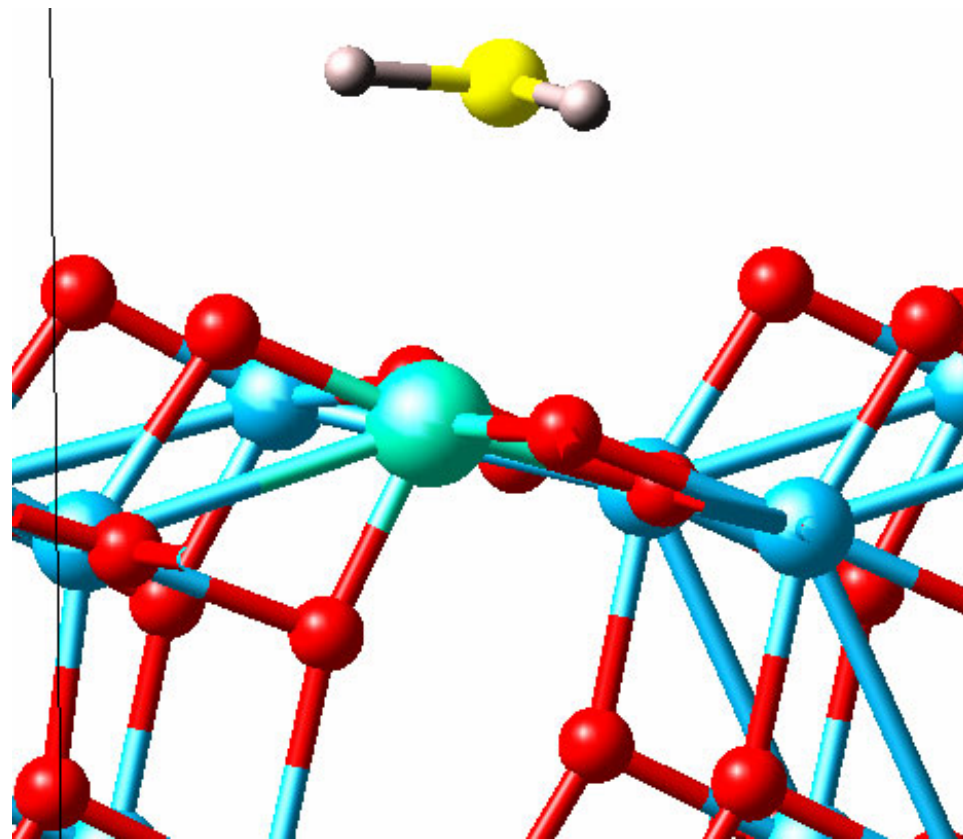
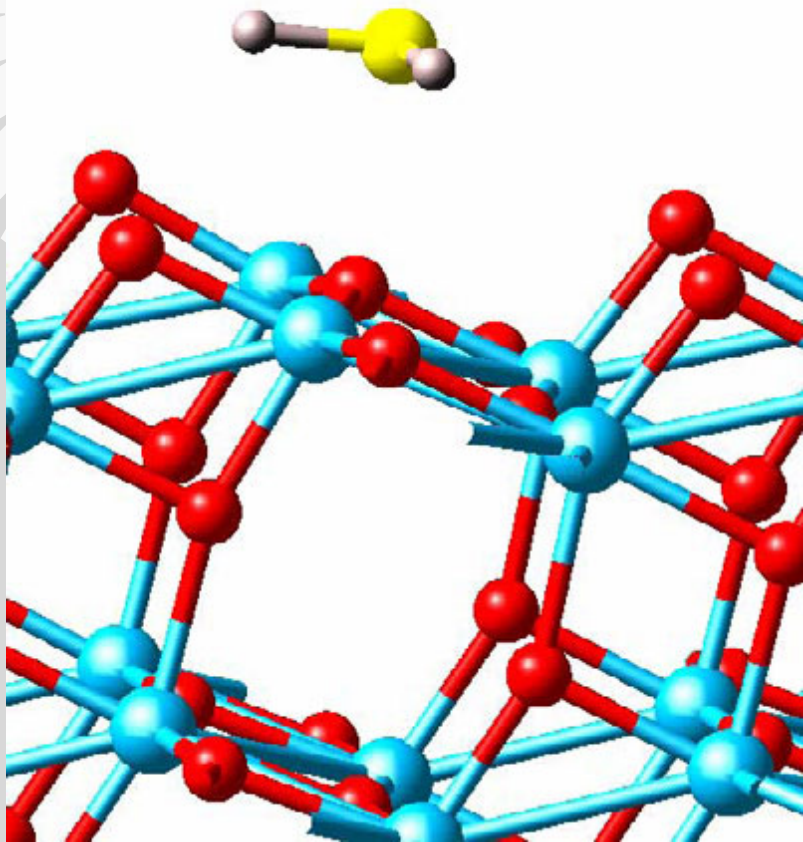


- $\text{Ce}_{0.5}\text{Zr}_{0.41}\text{Jr}_{0.09}\text{O}_2$ retains estimated 20% of 100 hr lined out activity after 40,000 hr at 400°C with 2 ppm S

- Oxide prepared on a multi-kg pilot plant scale had a surface area/skeletal oxide volume of $\sim 970 \text{ m}^2/\text{cm}^3$



H₂S Adsorption

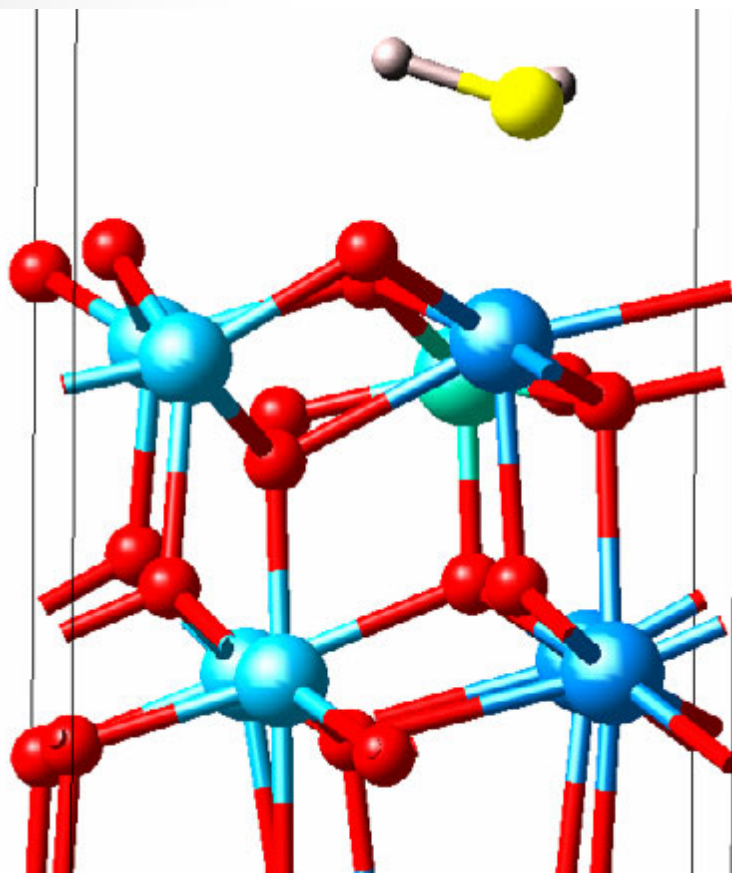


H₂S/TiO₂ Anatase(101)
Binding Energy: -1.93 eV/H₂S

H₂S/J6-Doped TiO₂ Anatase(101)
Binding Energy: -2.17 eV/H₂S

Ti J6 O H S

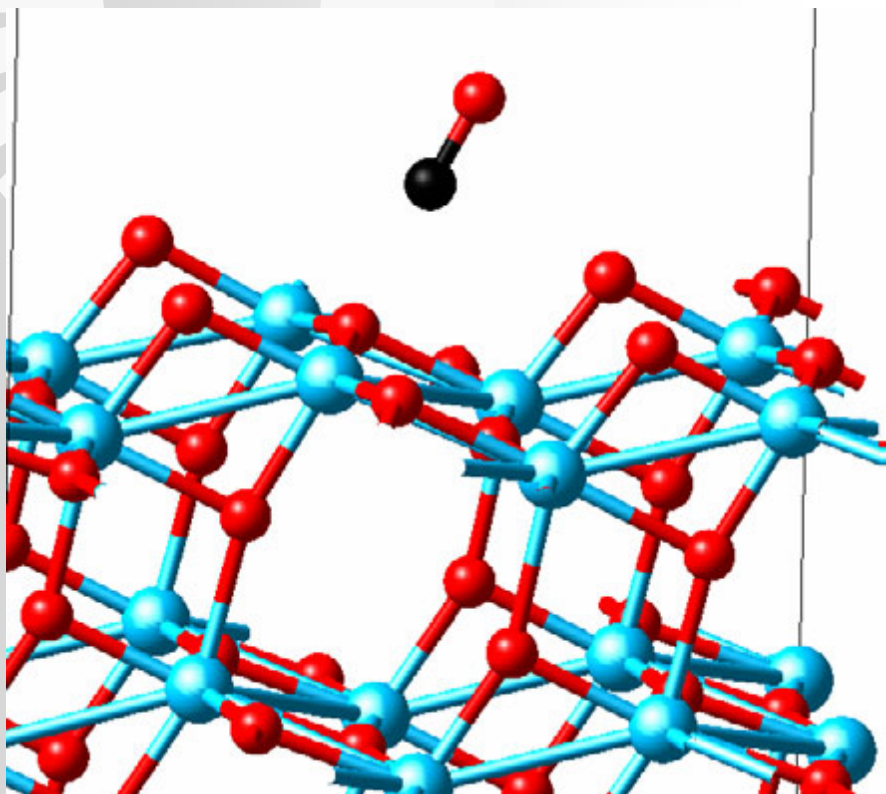
H₂S Adsorption



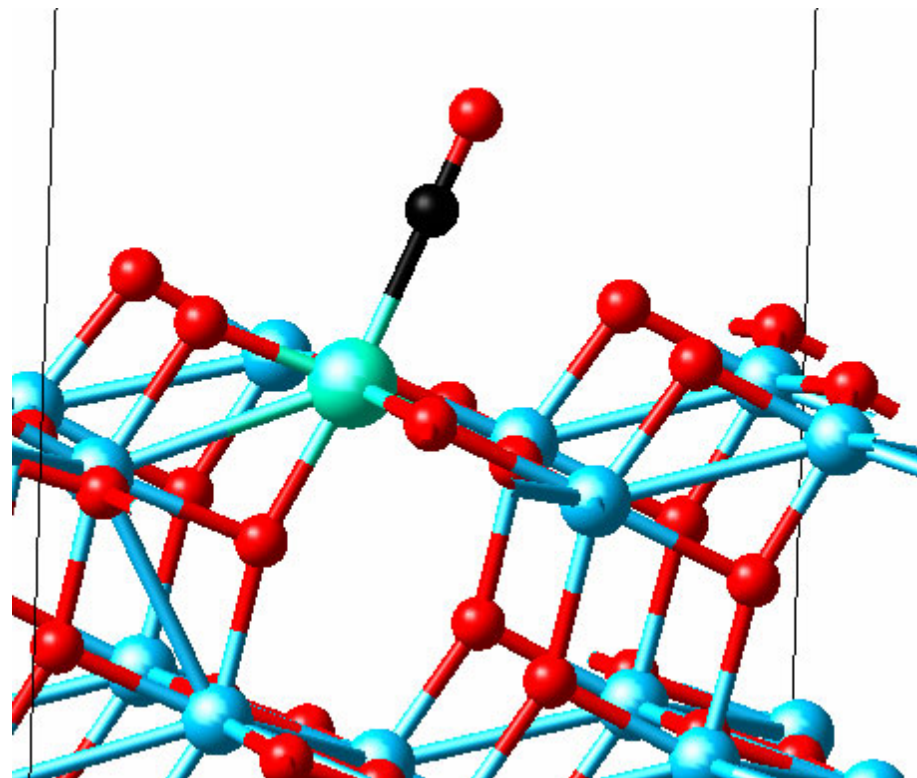
H₂S/Ce_{0.5}Zr_{0.42}J6_{0.08}O_x (111)
Binding Energy: -2.14 eV/H₂S

Ce Zr J6 O S H

CO Adsorption



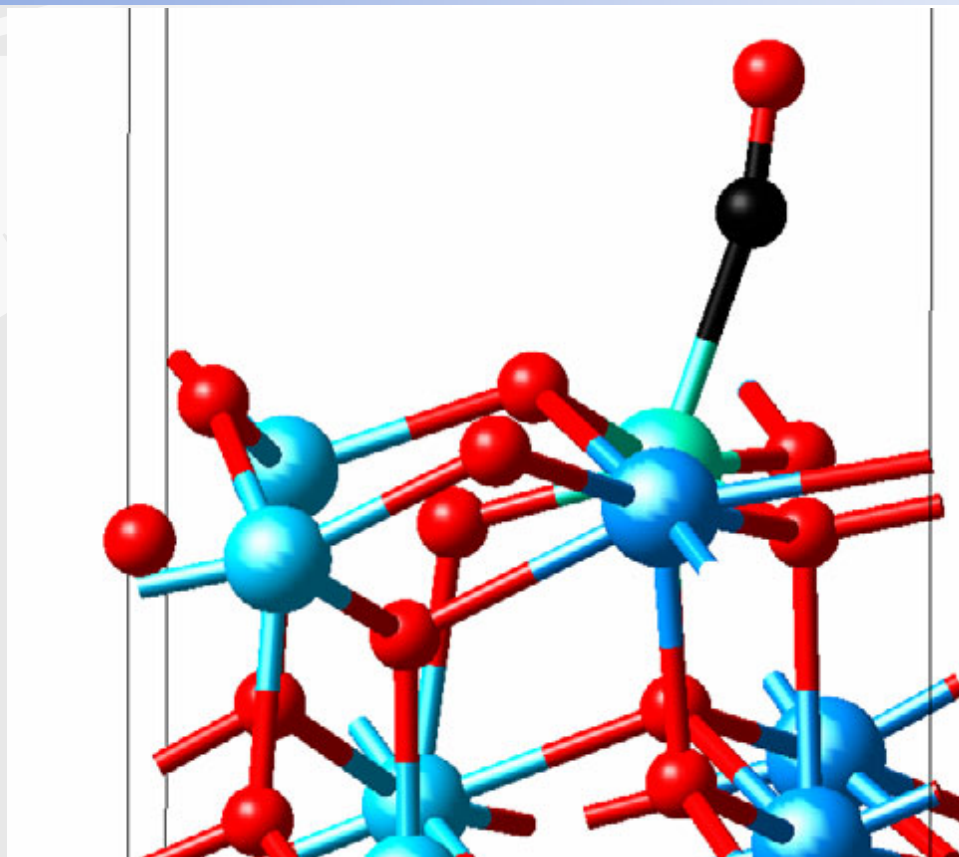
CO/TiO₂ Anatase(101)
Binding Energy: -0.32 eV/CO



CO/J6-Doped TiO₂ Anatase(101)
Binding Energy: -0.85 eV/CO

Ti J6 C O

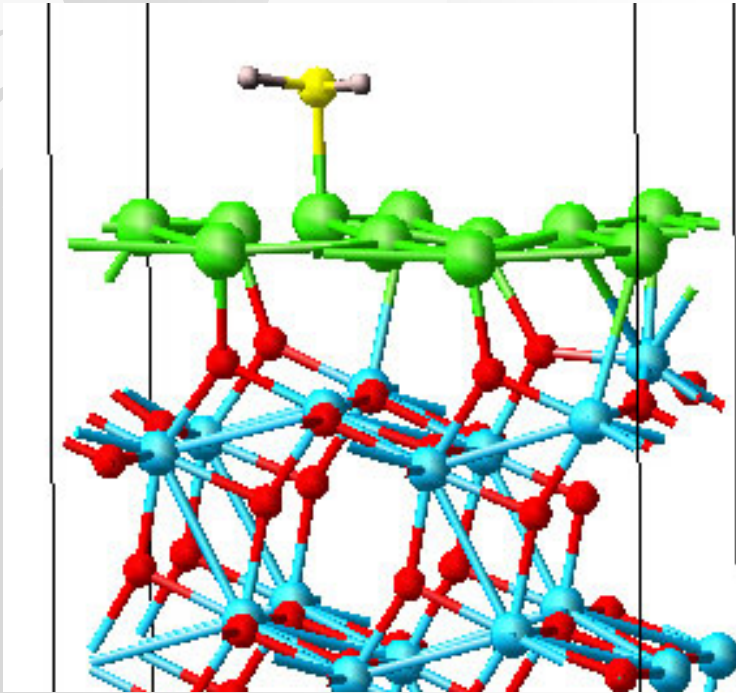
CO Adsorption



CO/Ce_{0.5}Zr_{0.42}J6_{0.08}O_x(111)
Binding Energy: -0.63 eV/CO

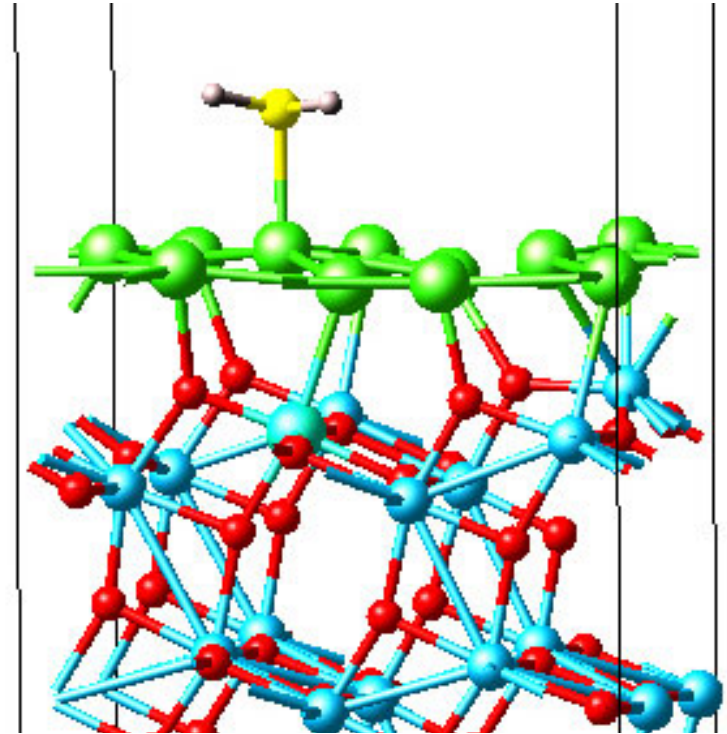
Ce Zr J6 O C

H₂S Adsorption (Pt ML)



H₂S/Pt_{1ML}/TiO₂Anatase(101)

Binding Energy:-0.76 eV/H₂S

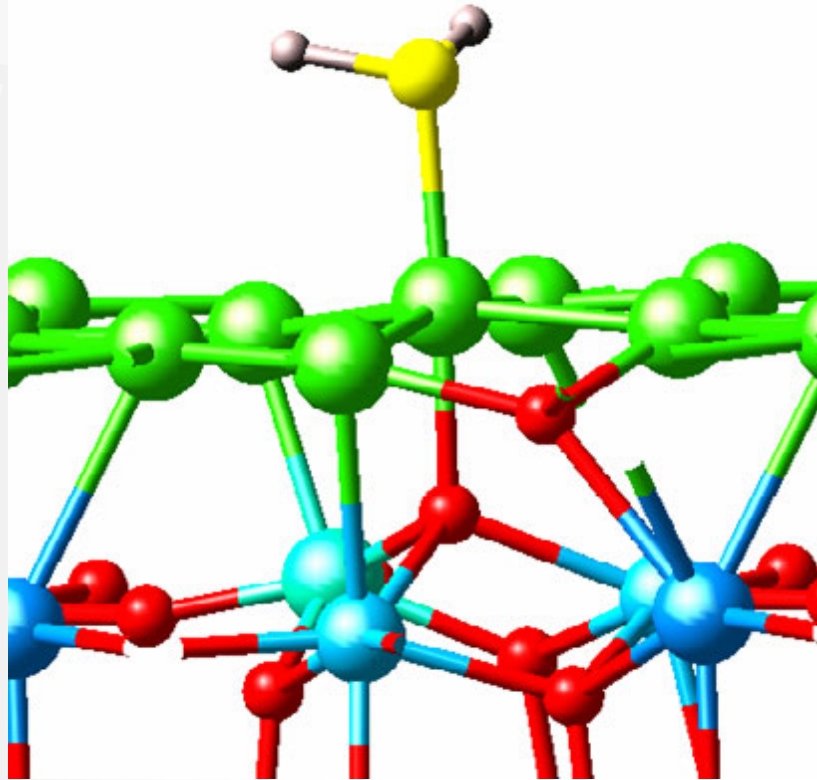


H₂S/Pt_{1ML}/J6-Doped TiO₂Anatase(101)

Binding Energy:-0.40 eV/H₂S

Pt O J6 Ti S H

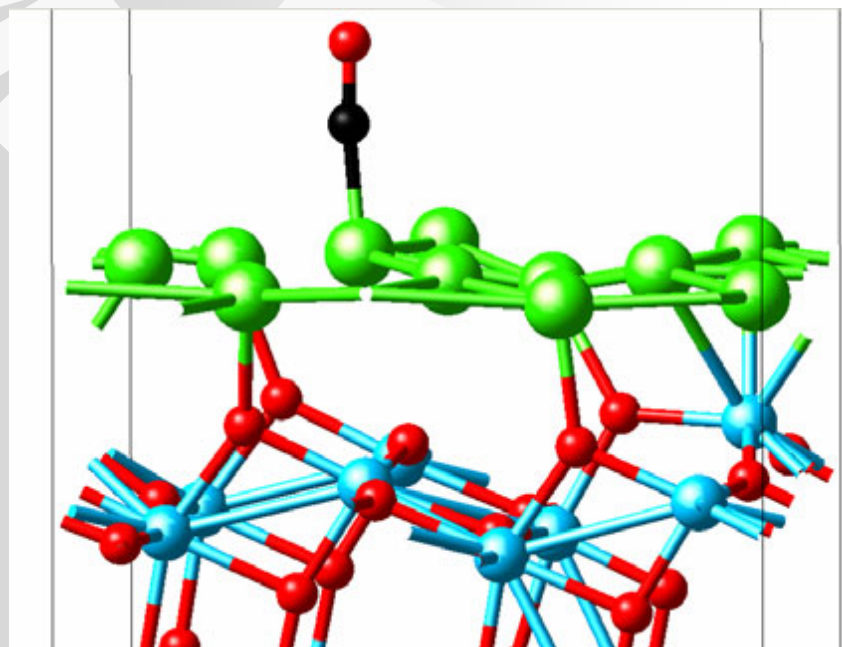
H₂S Adsorption (Pt ML)



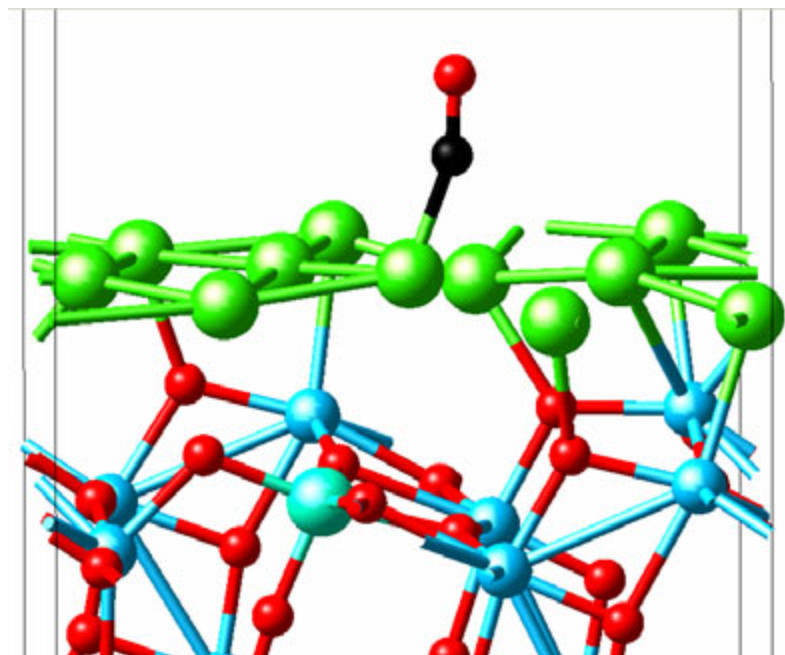
H₂S/Pt_{1ML}/ Ce_{0.5}Zr_{0.42}J_{6.08}(111)
Binding Energy: -2.04 eV/H₂S

Pt Ce Zr J6 O S H

CO Adsorption (Pt ML)



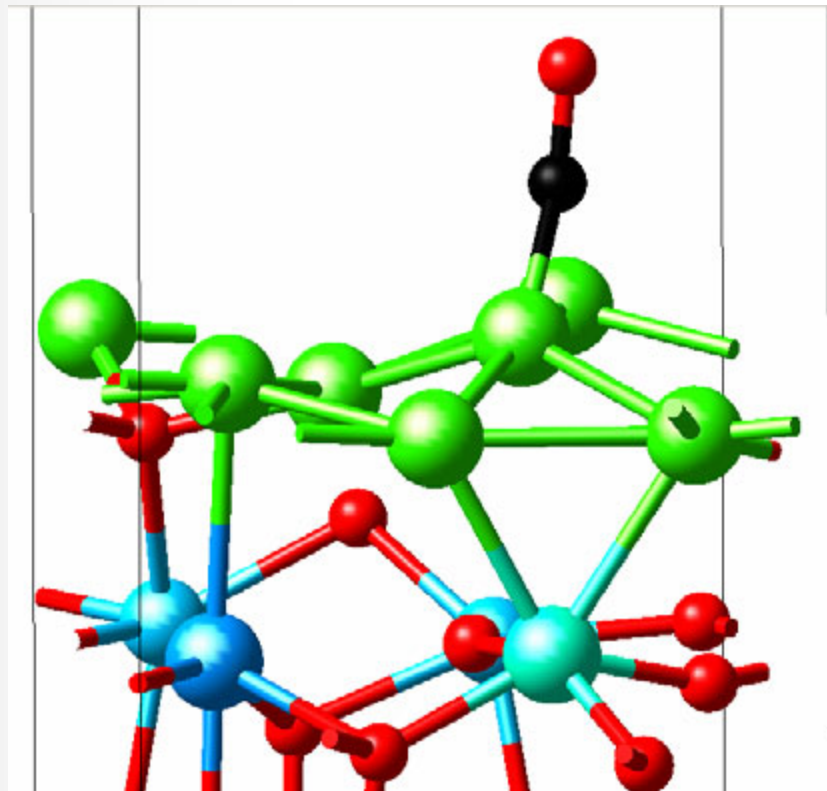
CO/Pt_{1ML}/TiO₂ Anatase(101)
Binding Energy: -1.67 eV/CO



CO/Pt_{1ML}/J6-Doped TiO₂ Anatase(101)
Binding Energy: -0.97 eV/CO

Pt Ti J6 C O

CO Adsorption (Pt ML)



$\text{CO/Pt}_{1\text{ML}}/\text{Ce}_{0.5}\text{Zr}_{0.42}\text{J6}_{0.08}\text{O}_x$
Binding Energy: -1.74 eV/CO

Pt Ce Zr J6 O C

Sulfur-free CO Conversion of WGS catalysts

Feed Conditions: 14% CO, 31% H₂O, 14.9% CO₂, 12% H₂

Feed Conditions: 7.5% CO, 31.6% H₂O, 7.9% CO₂, 6.4% H₂

