# NOVEL WATER GAS SHIFT CATALYSTS

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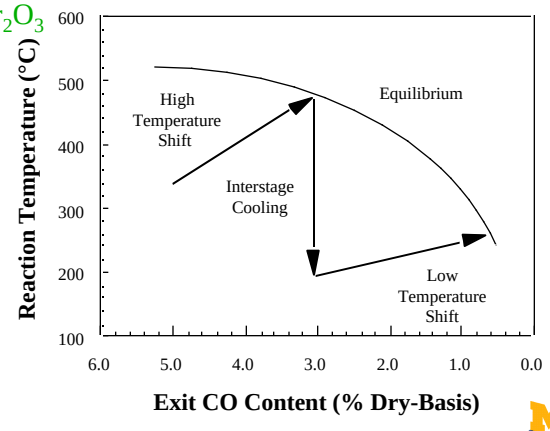
# Commercial Water Gas Shift (WGS)

$CO + H_2O \leftrightarrow CO_2 + H_2$ $\Delta H = -9.7$ kcal/mol

HTS Catalysts:
$Fe\text{-}Cr_2O_3$




LTS Catalysts:
$Cu\text{-}ZnO\text{-}Al_2O_3$

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# Candidate Catalysts

| Material | Price* ($ per lb.) | Relative Price |
|---|---|---|
| Ru | 1,116 | 159 |
| Rh | 14,050 | 2,007 |
| Pd | 5,515 | 788 |
| Ag | 66 | 9.4 |
| Ir | 5,468 | 781 |
| Pt | 6,827 | 975 |
| Au | 4,350 | 621 |
| $MoO_3$ | 3.86 | 0.6 |
| Cu/Zn/Al Catalyst | 7.00 | 1.0 |

* Prices in February, 2002.

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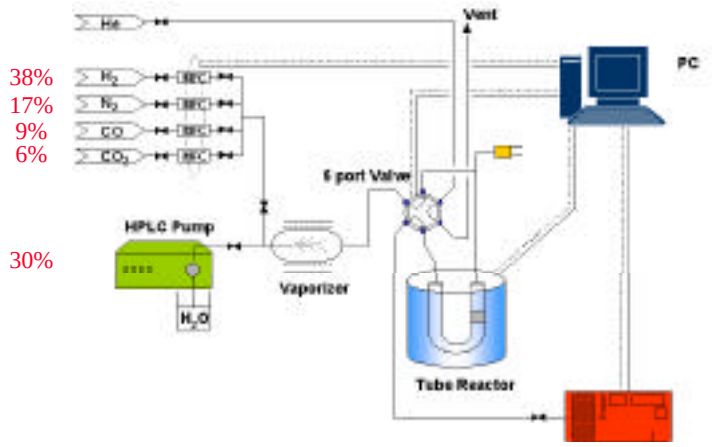
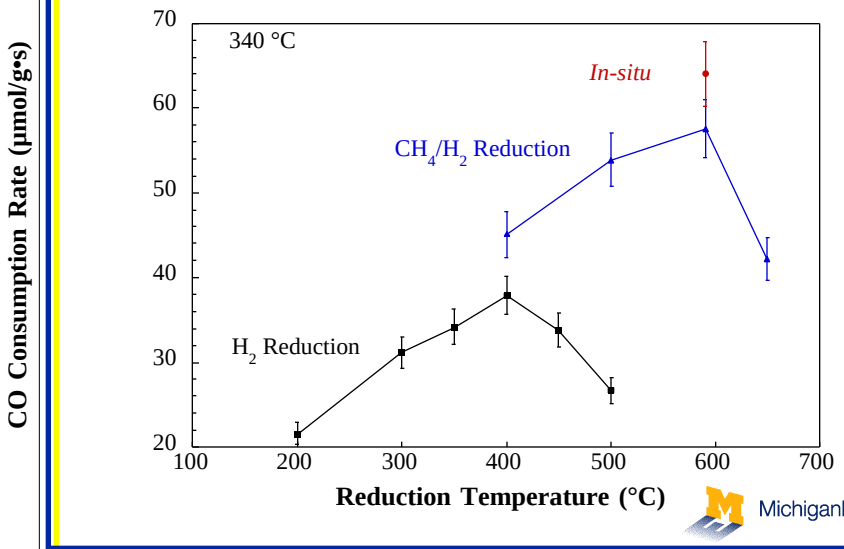
# WGS Micro-Reactor



# Effect of Pretreatment

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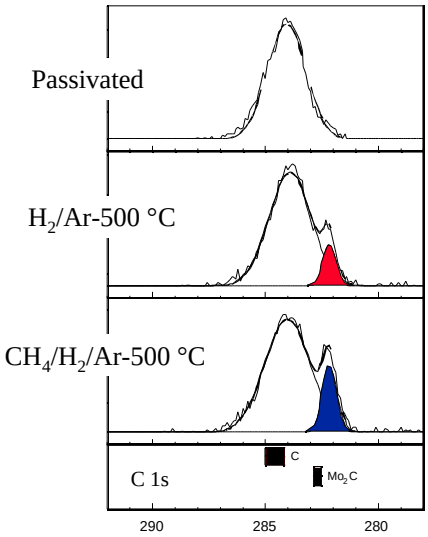
# Correlations?




| | Rate (µmol/gr/s) | Rate/ Peak Area | CO Uptake (ml/gr) | TOF (1/s) |
|---|---|---|---|---|
| $H_2$/Ar-500 °C | 16 | 1.7 | 3.3 | 0.11 |
| $CH_4/H_2$/Ar-500 °C | 34 | 2.2 | 6.0 | 0.12 |

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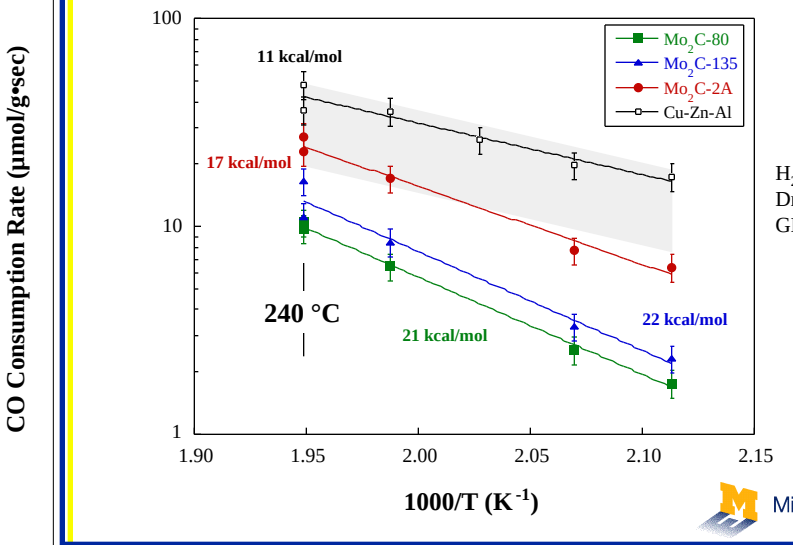
# $Mo_2C$ Catalysts




$H_2O$:CO=3.33
Dry gas=12% CO in $H_2$
GHSV≈300,000 $hr^{-1}$

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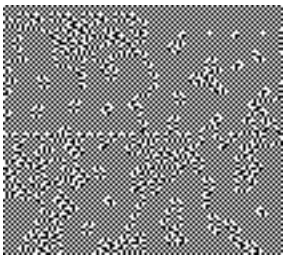
# Catalyst Options

Multimetallic Carbide



Carbide Supported Catalyst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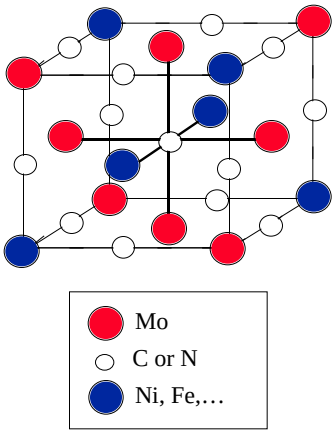
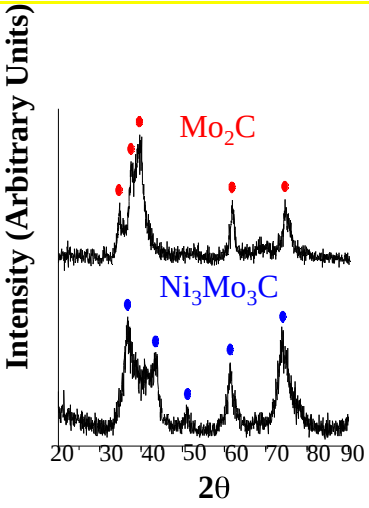
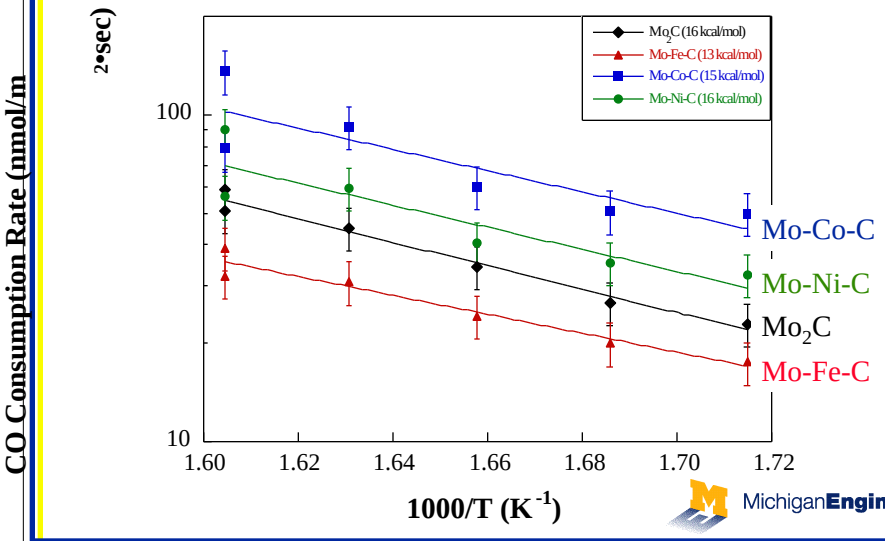
# η-Carbides




# Mo-M η-Carbides

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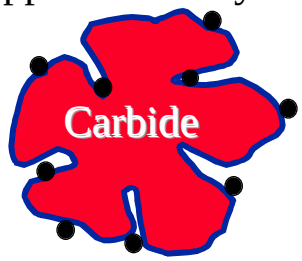
# $Mo_2C$-Supported Catalysts

Carbide Supported Catalyst


Oxycarbide or Oxide Supported Catalyst

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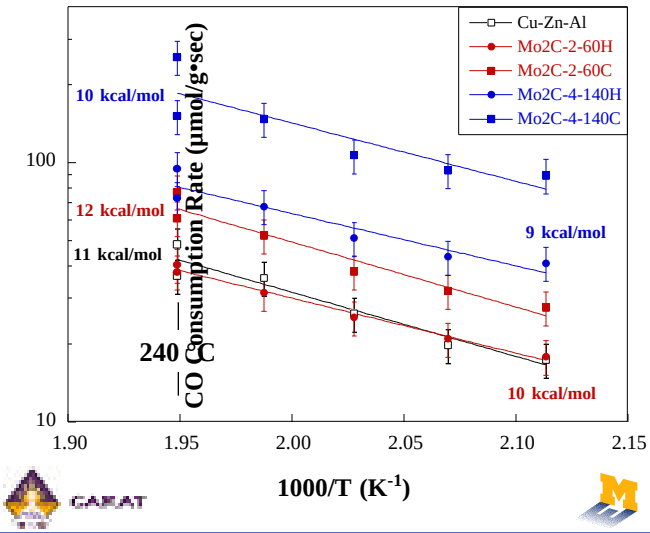
# $Mo_2C$-Supported Catalysts: Modified Method




$H_2O$:CO=3.33
Dry gas=12% CO in $H_2$
GHSV≈300,000 $hr^{-1}$

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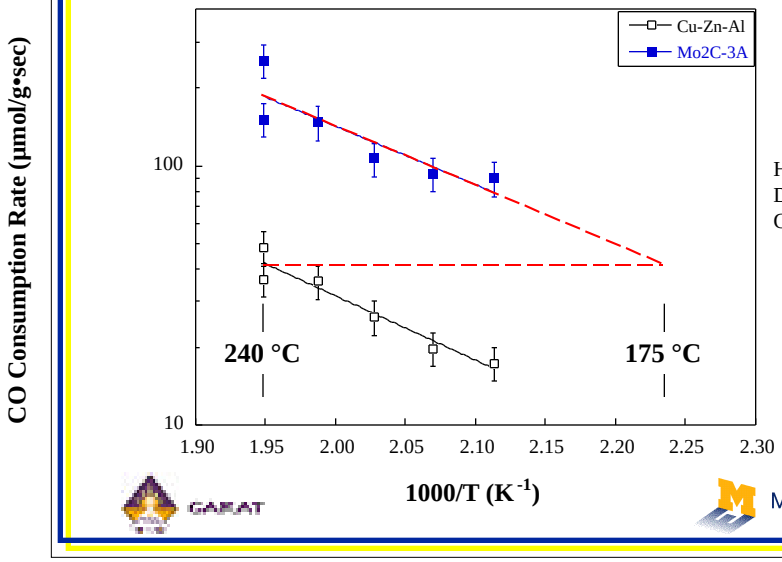
# Ultra-Low Temperature Shift




$H_2O$:CO=3.33
Dry gas=12% CO in $H_2$
GHSV≈300,000 $hr^{-1}$

GAPAT

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# Conclusions/Challenges

- Bulk carbides are highly active for WGS
- Reaction of CO and oxygen or hydroxyl appears to be RDS
- Carbide-supported catalysts hold promise for use in LTS and perhaps ULTS
- Reducible oxide supported Au catalysts can be highly active for WGS but they deactivate
- Introduction of textural promoters can help reduce deactivation

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# Acknowledgements


Research Group

- Novel Fuel Processing Catalysts
  - Jeremy Patt, Chang Kim, Easwar Ranganathan and Dr. Shyamal Bej
- Early Transition Metal Nitrides and Carbides
  - Randy McGee, Kamilah Turner and Yoshinori Kato and Dr. Chris Bennett
- Micro-Reactors and Micro-Fuel Cells
  - William Johnson, Tafaya Ransom, André Taylor, Dr. Hanwei Lei and Dr. Wen-Sheng Dong

Department of Energy and Honda Americas

Süd Chemie, Unicore, Catalyte

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