

## Heterogeneous catalysis – Catalysts database

This is a partial list of catalysts used in some industrially important heterogeneous catalytic reactions. The list will be updated gradually.

| Reaction  | Catalyst   | Remarks |
|---|--|---------|
| <b>Adsorption</b><br>Separation technology  | Polysiloxanes with various substitution groups<br><br>Packed catalyst columns  |         |
| <b>Adsorption</b><br>Water treatment  | Zeolites<br><br>Activated carbon   |         |
| <b>Adsorption</b><br>Air treatment  | Zeolites<br><br>Activated carbon   |         |
| <b>Alkylation</b><br><br>Benzene----> Toluene<br><br>Toluene----> Xylenes or styrene              | AlCl <sub>3</sub><br><br>Zeolite-X<br><br>Zeolite-Y<br><br>ZSM-5<br><br>Ag/Al <sub>2</sub> O <sub>3</sub><br><br>MCM-42<br><br>MCM-49<br><br>Pt/H-ZSM-5<br><br>La-Zeolite-X<br><br>SBA-15<br><br>H-MCM-22<br><br>CeO <sub>2</sub> -MgO |         |
| <b>Hydroformylation</b><br><br>CO+C <sub>n</sub> = +H <sub>2</sub> ---->C <sub>n+1</sub> aldehyde | Rh/Al <sub>2</sub> O <sub>3</sub><br><br>Rh/SiO <sub>2</sub>   |         |

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|   | <p>Rh/SiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub></p> <p>Pd/SiO<sub>2</sub></p> <p>Rh-Pd/SiO<sub>2</sub></p> <p>Rh-Co/SiO<sub>2</sub></p> <p>Au/Co<sub>3</sub>O<sub>4</sub></p> <p>Co/Al<sub>2</sub>O<sub>3</sub></p> <p>Co/SiO<sub>2</sub></p>                                     |  |
| <p><b>Hydrotreating – HDS</b></p> <p>R-SH+H<sub>2</sub>----&gt; R+ R<sup>≠</sup> + H<sub>2</sub>S</p>   | <p>Sulfided CoMo/Al<sub>2</sub>O<sub>3</sub></p> <p>Sulfided NiMo/Al<sub>2</sub>O<sub>3</sub></p>   | Industrial catalyst                                    |
| <p><b>Hydrotreating – HDN</b></p> <p>R-NH<sub>2</sub>+H<sub>2</sub>----&gt; R+ R<sup>≠</sup> + NH<sub>3</sub></p>   | <p>Sulfided NiMo/Al<sub>2</sub>O<sub>3</sub>,<br/>Pd/Al<sub>2</sub>O<sub>3</sub></p>  |  |
| <p><b>Epoxidation</b></p> <p>CH<sub>2</sub>=CH<sub>2</sub>----&gt; (CH<sub>2</sub>-CH<sub>2</sub>)O</p> <p>CH<sub>2</sub>=CH-CH<sub>3</sub>-----&gt;</p> <p>(CH<sub>2</sub>-CH-CH<sub>3</sub>)O</p>                   | <p>Ag, Ag/Au supported on zeolites, carbonates (CaCO<sub>3</sub>, MgCO<sub>3</sub>, SrCO<sub>3</sub>, BaCO<sub>3</sub>), CaF, CaTiO<sub>2</sub>, tribasic calcium phosphate, calcium molybdate, magnesium molybdate, strancium molybdate</p>  | Catl. Lett.: 2002, 80, 93                              |
| <p><b>Selective hydrogenation</b></p> <p>1,3-butadiene</p> <p>α,β-unsaturated aldehydes</p> <p>Crotonaldehyde----&gt;</p> <p>Crotyl alcohol</p> <p>3-methyl crotonaldehyde----&gt;</p> <p>3-methyl crotyl alcohol</p> | <p>Lindlar catalyst</p> <p>Pd/CaCO<sub>3</sub> with Pb/Bi or Amine/Sulfur</p> <p>Al<sub>2</sub>O<sub>3</sub> supported catalysts of Fe, Co(10%), Ni, Cu(10%), or Pd(5%)</p> <p>Al<sub>2</sub>O<sub>3</sub> supported catalysts of Cu, Ni, Fe</p> <p>Ru, Re, Os supported on ZnO</p> | <p>Pharma, Perfumes, Flavors</p> <p>Batch reactors</p> |

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|   | <p>Pt (promoted by Fe or Sn)/SiO<sub>2</sub> with Pt:Sn 4:1</p> <p>Cu or Cu(sulfidation) /Al<sub>2</sub>O<sub>3</sub></p> <p>Cu/SiO<sub>2</sub></p> <p>Cu-Pd (3:1)</p> <p>Pt/TiO<sub>2</sub></p>  |  |
| <p><b>Selective oxidation</b></p> <p>Propylene glycol----&gt; acids</p> <p>aldehydes, ketones</p> <p>Glycerol oxidation</p>   | <p>Pt, Pd (promoted by Bi or Pb)</p> <p>Supported on C or Al<sub>2</sub>O<sub>3</sub></p> <p>Also: Cd, Co, Cu, Se, Ce, Te, Sn, Au, Ru serve as promoters</p> <p>Pt, Pd, Au, or Ag supported on C, graphite, pumice</p> <p>Also: PdAg/Pumice</p> |  |
| <p><b>CO oxidation</b></p> <p><b>Water gas shift reaction</b></p> <p><b>DeSox</b></p> <p><b>Complete oxidation of CH<sub>4</sub></b></p> <p><b>Selective partial oxidation of propene</b></p> <p><b>Olefin hydrogenation</b></p> <p><b>NO reduction with hydrocarbons</b></p> | <p>All these reactions utilize:</p> <p>Au/CeO</p> <p>Au/TiO<sub>2</sub></p> <p>Au/TiC</p> <p>(Ceria, oxides, carbides titania serve as good supports)</p>   |  |
| <p><b>Enantio selective reaction</b></p>  | <p>Adams Pt catalyst</p> <p>Pt/Cinchona</p> <p>2.5%Pt/SiO<sub>2</sub></p> <p>Pt/Al<sub>2</sub>O<sub>3</sub></p>   |  |

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| <p><b>DeSOx</b></p> <p>Decomposition of SO<sub>2</sub></p> <p>SO<sub>2</sub>+2H<sub>2</sub>S-----&gt; 2H<sub>2</sub>O+3S</p>   | <p>Au/TiO<sub>2</sub></p>   |   |
| <p><b>Fischer Tropsch (FT) process</b></p> <p>CO+H<sub>2</sub>--&gt; Hydrocarbons</p> <p style="padding-left: 40px;">C-C compounds</p> <p>In general:</p> <p>nCO+nH<sub>2</sub>----&gt; (-CH<sub>2</sub>-)<sub>n</sub> + nH<sub>2</sub>O</p> | <p>Fe and Co based catalysts with Ru, Cu, Ni and K<sub>2</sub>O promotion (Sasol reaction)</p> <p>Fe/ZrO<sub>2</sub></p> <p>Fe/K/ZrO<sub>2</sub></p> <p>Co/SiO<sub>2</sub> (FT Catalyst)</p> <p>Fe-H-ZSM-5</p> <p>0.5%La promoted using La<sub>2</sub>O<sub>3</sub></p> <p>On 15%Co/Activated carbon</p> <p>Co/Al<sub>2</sub>O<sub>3</sub></p> <p>Ru/Co/ZrO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub></p> <p>CoRe/Al<sub>2</sub>O<sub>3</sub></p> | <p>Low Temp FT uses Co</p> <p>High Temp FT uses Fe</p> <p>Promotes alcohol formation</p>  |
| <p><b>Methanol synthesis</b></p> <p>CO/CO<sub>2</sub>/H<sub>2</sub>-----&gt; CH<sub>3</sub>OH</p> <p>CO+2H<sub>2</sub>-----&gt; CH<sub>3</sub>OH</p>   | <p>Cu/ZnO/Al<sub>2</sub>O<sub>3</sub></p> <p>Cu-Zn</p> <p>Cu/SiO<sub>2</sub>-Zr</p> <p>Cu/ZrO<sub>2</sub></p> <p>Cu/ZnO</p> <p>Pd/SiO<sub>2</sub></p> <p>Pd/ZrO<sub>2</sub></p> <p>Pd/TiO<sub>2</sub></p>   | <p>EtOH product</p> <p>(C-C product formation)</p> <p>Hydrocarbons (HC) formation</p> <p>EtOH formation</p> <p>C<sub>2</sub> oxygenates</p> |

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|   | <p>Ca-Pd/SiO<sub>2</sub></p> <p>Cs-Cu/ZnO/Al<sub>2</sub>O<sub>3</sub></p> <p>Rh/SiO<sub>2</sub></p> <p>Rh/Al<sub>2</sub>O<sub>3</sub></p> <p>Rh/ZrO<sub>2</sub> or TiO<sub>2</sub> or CeO<sub>2</sub> or MnO or La<sub>2</sub>O<sub>3</sub></p> <p>Rh/SiO<sub>2</sub> promoted by Mn/Fe/Li or Nb</p> |  |
| <p><b>Hydrogenation</b></p> <p>Alkene-----&gt; alkane</p> <p>Acids-----&gt; alcohols</p> <p>Esters-----&gt; alcohols</p> <p>Oils and fats</p> | <p>Ru/C, Pd/C</p> <p>Ru/C, Pd/C, Pt/C</p> <p>Cu/SiO<sub>2</sub>, copper chromite, Ba promoted copper chromite</p> <p>Supported Ni</p>  |  |
| <p><b>Dehydrogenation</b></p> <p>Alkane dehydrogenation</p>   | <p>Supported ZSM-5</p> <p>Ga/ZSM-5</p> <p>Pt/Mg(Ga)(Al)O</p> <p>Pt/Fe/ZSM-5</p> <p>Pt/Mg(In)(Al)O</p> <p>V<sub>2</sub>O<sub>5</sub>/MCM-41</p> <p>V/Al<sub>2</sub>O<sub>3</sub></p> <p>CrO<sub>x</sub>/SiO<sub>2</sub></p> <p>Pd/Al<sub>2</sub>O<sub>3</sub></p> <p>Supported Cr catalysts</p>       |  |
| <p><b>Oxidation</b></p> <p>Partial oxidation of alkanes</p>   | <p>Fe/SiO<sub>2</sub></p>  |  |

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|  | <p>PdV/TiO<sub>2</sub></p> <p>Ti-Beta</p> <p>V/MCM-41</p> <p>Pt/Al<sub>2</sub>O<sub>3</sub></p> <p>Rh/Al<sub>2</sub>O<sub>3</sub></p> <p>Mn-Zeolite-5, 55, 58</p> <p>Ti-Silicates</p> <p>Pt/Mg(Ga)(Al)O</p> <p>V<sub>2</sub>O<sub>5</sub></p> <p>V<sub>2</sub>O<sub>5</sub>/TiO<sub>2</sub></p> |                 |
| <b>Ammonia synthesis</b>   | <p>Os</p> <p>Ur</p> <p>Fe promoted with K<sub>2</sub>O, CaO, SiO<sub>2</sub>, and Al<sub>2</sub>O<sub>3</sub></p> <p>Ru/C</p> <p>Co/C</p> <p>Ba-Fe-Co/C</p> <p>Ru/MgO</p>   |                 |
| <p><b>CO<sub>2</sub> hydrogenation</b></p> <p>CO<sub>2</sub>+H<sub>2</sub>-----&gt; CO, HCOOH, HCHO, CH<sub>3</sub>OH</p> <p>CO<sub>2</sub>+CH<sub>4</sub>-----&gt; 2CO+2H<sub>2</sub></p> | <p>Cu-Zn-chromite</p> <p>H-zeoliteY</p> <p>ZrO<sub>2</sub> – good support for high temperature hydrogenation</p> <p>Pt(Sn)/SiO<sub>2</sub></p> <p>Fe(K, Cu)/Al<sub>2</sub>O<sub>3</sub></p>   | Dry reformation |

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| <p><b>CH4 Partial oxidation</b></p> <p>CH4-----&gt; CH3OH or<br/>HCO species</p> <p>Oligomerization</p> <p>Dimerization</p> <p>Partial oxidation</p> <p><b>Dry reforming of CH4</b></p> | <p>Ru/TiO2</p> <p>Ru/SiO2</p> <p>Ru/Al2O3</p> <p>Pt/CeZrO2/Al2O3</p> <p>Ni or Ni-Au/MgO-Al2O3</p> <p>Ni/Al2O3-aluminium nitride</p> <p>Ni/SiO2</p> <p>Ni/Mg(Al)O</p> <p>Ni/MCM-41</p> <p>Re/Al2O3</p> <p>Mg-Al LDH</p> <p>Ru/SiO2</p> <p>Ru/Al2O3</p> <p>Ru/C</p> <p>Pt/Al2O3</p> <p>Ni/Al2O3</p> <p>PtNi/Al2O3</p> <p>Rh/Al2O3</p> <p>Rh/La2O3</p> <p>NiCu/SiO2</p> |                           |
| <p><b>Methanol to Hydrocarbons (MTG)</b></p> <p>CH3OH-----&gt; C2-C9<br/>hydrocarbons</p>   | <p>H-ZSM-5</p> <p>Cu/SiO2</p> <p>Raney-Ni</p>  | <p>Dimethyl carbonate</p> |

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|   | Cu+zeolite-X  |   |
| <b>Steam reforming</b><br>$\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$  | Ni on $\text{Al}_2\text{O}_3$ or $\text{MgO}$ promoted<br>with Au, Ag, Sn, Cu, M, Fe, Ru<br>and other transition metals<br><br>Cu/ZnO   |   |
| <b>Water gas shift (WGS) reaction</b><br>$\text{CO} + \text{H}_2 \rightarrow \text{CO}_2 + \text{H}_2$  | CuO-ZnO- $\text{Al}_2\text{O}_3$<br><br>$\text{Fe}_2\text{O}_3$ - $\text{Cr}_2\text{O}_3$ - $\text{MgO}$<br><br>Au/ $\text{CeO}_2$ or $\text{TiO}_2$<br><br>Cu/ $\text{CeO}_2$  |   |
| <b>Hydrogen production</b><br><br><b>(Steam reforming followed by WGS process)</b><br><br>$\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$<br><br>$\Delta H = + 206 \text{ kJ/mol (298K)}$<br><br>Favored at high T and low P<br><br>Then do WGS:<br><br>$\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$<br><br>$\Delta H = - 41 \text{ kJ/mol (298K)}$ | Supported Ni catalyst<br><br>(Noble metals as activators)<br><br>High T shift:<br><br>$\text{Fe}_2\text{O}_3/\text{Cr}_2\text{O}_3$ at 670K<br><br>Low T shift:<br><br>Cu/ZnO at 470K<br><br>Ni/MgO<br><br>Ni/YSZ<br><br>Sn/Ni/YSZ<br><br>Ni/MgO/alkali<br><br>Pd/ $\text{CeO}_2/\text{Al}_2\text{O}_3$<br><br>Ni/MgO<br><br>Ni/ $\text{TiO}_2$<br><br>Pt/ $\text{TiO}_2$<br><br>Pt/ $\text{ZrO}_2$ | 700 - 1250K / 30 bar<br><br>TOF = $0.5 \text{ s}^{-1}$ at 723K<br><br>(with 10% $\text{CH}_4$<br>conversion)<br><br>Coking should be<br>controlled<br><br>Steam dissociation<br><br>$\text{CO}_2$ reforming |

|                              |                                      |  |
|------------------------------|--------------------------------------|--|
|                              | Ag-Ni/Al <sub>2</sub> O <sub>3</sub> |  |
|                              | Co-Ni/ZrO <sub>2</sub>               |  |
| <b>Methanol to Aromatics</b> | Impregnated Zeolites                 |  |
|                              | Ni/ZSM-5                             |  |
|                              | Cu/ZSM-5                             |  |
|                              | Zn/ZSM-5                             |  |
|                              | Ga/ZSM-5                             |  |
|                              | Ir/ZSM-5                             |  |
|                              | Ru/ZSM-5                             |  |
|                              | Pd/ZSM-5                             |  |
|                              | Ag/ZSM-5                             |  |

### **References:**

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