Photooxidation of isopropanol

\[
\text{(CH}_3\text{)}_2\text{CHOH} \rightarrow \text{(CH}_3\text{)}_2\text{C}=\text{O} + 2\text{H}^+ + 2\text{e}^-
\]

\[
2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2
\]

**Light**

\(\lambda > 425\text{ nm}\)

60 mW/cm\(^2\)

Dr. Gonghu Li
Dr. Christiaan Richter

CHEM 505: Green Chemistry and Alternative Energy
Crabtree – Brudvig – Schmuttenmaer – Batista
Department of Chemistry – Yale University

Modeling Systems for a Hydrogen Economy
Photocatalysis with Visible Light
Modeling Systems for a Hydrogen Economy

Photocatalysis with Visible Light

Dr. Gonghu Li
Dr. Christiaan Richter

Net redox reaction:

\[(\text{CH}_3)_2\text{CHOH} \xrightarrow{hv} (\text{CH}_3)_2\text{C}=\text{O} + \text{H}_2\]

\(\text{TiO}_2/\text{Mn-cat.}\)

Photoactivation of the catalyst:

Photooxidation of isopropanol
At equilibrium: $E_F = \mu_L = \mu_R$

**Molecular Rectification:** DFT NEGF: I-V Characteristics
**Molecular Rectification:** DFT NEGF: I-V Characteristics
**Molecular Rectification:** DFT NEGF: I-V Characteristics
DFT-NEGF Methodology

\[ \hat{H} = \begin{pmatrix} H_L & V_{LD} & 0 \\ V_{LD}^* & H_D & V_{RD}^* \\ 0 & V_{RD} & H_R \end{pmatrix} \]

\[ \Sigma_{L/R} = (E_{S_{LD/RD}}^+ - V_{L/R}^+) g_{L/R} \left( E_{S_{LD/RD}} - V_{L/R} \right) \]

\[ \hat{H} \rightarrow \hat{G} = \left( E\hat{S} - \hat{H} - \hat{\Sigma} \right)^{-1} \rightarrow T(E) = Tr\left( \hat{\Gamma}_L \hat{G}_D \hat{\Gamma}_R \hat{G}_D^* \right) \rightarrow \text{Current: } I \]

\[ \hat{\Sigma} = \hat{\Sigma}_L + \hat{\Sigma}_R \]

\[ G_D = \left( E S_D - H_D - \Sigma_L - \Sigma_R \right)^{-1} \]

\[ \Gamma_{L/R} = i \left( \Sigma_{L/R} - \Sigma_{L/R}^+ \right) \]

\[ I = \frac{2e}{\hbar} \int_{-\infty}^{\infty} dE \ T(E) \left[ f_L(E) - f_R(E) \right] \]

\[ \approx \frac{2e}{\hbar} \int_{\mu_L}^{\mu_R} dE \ T(E) \]

Wendu Ding – Christian Negre

Yale University
Wendu Ding, Leslie Vogt, Christian F. A. Negre, and Victor S. Batista
Molecule-Lead coupling

HOMO (D)  LUMO (A)  Fermi Level

Wendu Ding, Leslie Vogt, Christian F. A. Negre, and Victor S. Batista
Single Frontier Orbital Mechanism

V=0

V>0

V<0

Wendu Ding, Leslie Vogt, Christian F. A. Negre, and Victor S. Batista
4,4’-Diaminostilbene

H₂N—\(\text{C}═\text{C}\)\—NH₂

---

**Figure 3.** Nanotechnology. 2009, 20, 434009

**Prof. Latha Venkataraman**
Columbia University

---

**Wendu Ding**
Yale University
Molecular Rectification:
The Break Junction Technique & Recent Results

11-1-2013
Chris Koenigsmann
Molecule R5

1. Well defined single molecule conductance plateaus (A).
2. Conductance $\sim 2.9 \times 10^{-4} G_0$
3. Small but measureable increase in conductance as bias increases.
4. A second low-conductance plateau (B) also observed (+400 mV).
Experimental and Theoretical IV curves

RR@0.85V = 1.3

RR@0.85V = 1.33

Latha Venkataraman, Chris Koeningsmann (I-V exp), Matthieu Koepf (synthesis), Christian Negre (I-V calc)
R5, Rectification at 0.85 V = 1.45

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Conductance ($G_0$)</th>
<th>RR</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>$1.7 \times 10^{-4}$</td>
<td>1.30</td>
</tr>
<tr>
<td>R5</td>
<td>$2.9 \times 10^{-4}$</td>
<td>1.45</td>
</tr>
</tbody>
</table>
Examples of Rectifying & Poor-Rectifying Molecules

![Molecules 1, 2, and 3 with Au terminals](image)

Scaled, statistically most probable IV curves for the three molecules. The curves are calculated from log-binned 2D histograms with bin sizes and histogram ranges kept constant. All curves have been scaled to zero-bias conductance of molecule 3, with the red curve multiplied by 2 and the blue curve by 4. Inset: Rectification ratio as a function of bias. Molecule 3 rectifies over three times as much as molecule 2, with rectification at 0.85V approaching 2.
Modeling Systems for a Hydrogen Economy

Molecular Inverse Design: LCAP Methodology

**Schrödinger equation in EH matrix form is**

\[ \mathbf{H} \mathbf{C} = \mathbf{E} \mathbf{S} \mathbf{C} \]

- **Hamiltonian matrix**
- **Eigenvector matrix** (diagonal matrix)
- **Overlap matrix** (AO basis set)

**LCAP-EHTB:**

**Diagonal terms**

\[ H_{ii}^{(\text{var})} = \sum_{A=1}^{N_{\text{type}}} b_A^i h_{ii}^{(A)} \]

**Off-diagonal terms**

\[ H_{ij} = \sum_{A=1}^{N_{\text{type}}} \sum_{A'=1}^{N_{\text{type}}} b_A^i b_{A'}^j h_{ij}^{(A,A')} \]

**Example:**

**S-orbital**

\[ \begin{array}{c}
\text{O} \\
1 \\
2 \\
\text{C, O}
\end{array} \]

**P\text{\_x}-orbital**

**Diagonal term**

\[ H_{22}^{P_x} = b_C^2 \cdot h_{22}^{(C_x)} + b_O^2 \cdot h_{22}^{(O_x)} \]

**Off-diagonal term**

\[ H_{12}^{SP_x} = b_O^1 \cdot b_C^1 \cdot h_{12}^{(O_x,C_x)} + b_O^1 \cdot b_O^2 \cdot h_{22}^{(O_x,O_x)} \]
Target molecular property: the total visible absorbance

\[ f = \sum_{p,q} f_{pq} \quad + \text{constraint: } 400 \text{nm} \leq \lambda_{pq} \leq 800 \text{nm} \]

\( f_{pq} \) is the oscillator strength of the \( p \) to \( q \) electronic transition, and \( \lambda_{pq} \) is the wavelength of the electronic transition.

\[
f_{pq} = \frac{8\pi^2 \nu_{pq} m_e}{3\hbar^2} |\mu_{pq}|^2
\]

\( \mu_{pq} = \langle \psi_q | r | \psi_p \rangle \): transition dipole moment,

\( \nu_{pq} \): wavenumber of the electronic transition,

\( m_e \): electron mass.

Gradients of molecular property:

\[
\frac{\partial f}{\partial b_A^i} = \frac{f(+\delta b_A^i) - f(-\delta b_A^i)}{2\delta b_A^i}
\]

Finally, the continuous optimization of \( f \) by varying \( \{b_A^i\} \) is performed based on a quasi-Newton (BFGS algorithm) method.
Modeling Systems for a Hydrogen Economy

Inverse Design: Molecular Sensitizers

Dr. Dequan Xiao

TiO$_2$
Modeling Systems for a Hydrogen Economy
Inverse Design: Molecular Sensitizers

CHEM 505: Green Chemistry and Alternative Energy
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Department of Chemistry – Yale University

Dr. Dequan Xiao
Modeling Systems for a Hydrogen Economy

Liquid H-Carriers: Fuel Cell/Flow Battery Concept

Thermal (de)hydrogenation

![Chemical Reaction](image)

“Feed the hydrogenated organic liquid carrier directly into the fuel cell where it is electrochemically dehydrogenated without ever generating $H_2$”
Electrochemical dehydrogenation can be done at lower temperatures and high rates.

**Chemical Equations**

1. \[ \text{LQ} + \text{H}_2 \rightarrow \text{LQ} + \text{H}_2 \text{O} + n \text{e}^- \]
2. \[ \frac{n}{2} \text{O}_2 + n \text{H}_2 \text{O} \rightarrow \frac{n}{2} \text{H}_2 \text{O} + n \text{e}^- \]
3. \[ \text{LQ} + \frac{n}{2} \text{O}_2 \rightarrow \text{LQ} + \frac{n}{2} \text{H}_2 \text{O} \]

*where LQ stands for an organic carrier molecule*

Electrochemical dehydrogenation of saturated cyclic hydrocarbons (e.g., cyclohexane and decaline) is possible in alkaline electrolyte using Pd and Rh catalysts.

Temperature (K) for spontaneous (de)hydrogenation $\Delta G = 0$ (DFT B3PW91).

Exercise 4:

Nitrogen atoms introduced into heterocycles tune the thermodynamic tendency to absorb or release H$_2$, or to absorb or release 2(H$^+$ and e$^-$). A particularly favorable condition is when aromatic stabilization can be achieved after cleavage of only four C-H bonds as in the following reaction:

\[
\text{Pyridine} \rightarrow \text{Pyridazine} -2\text{H}_2
\]

This can be analyzed by computing the temperature $T = T_d$ that makes the dehydrogenation free energy $\Delta G = \Delta H - T \Delta S$ equal to zero. At this point ($T = T_d$) the unfavorable enthalpy due to the endothermicity of the reaction is exactly compensated by the favorable entropy of H$_2$ release.

(a) Find the minimum energy configurations of reactants and products for the dehydrogenation reaction shown above in the gas-phase at the DFT B3PW91 level of theory.

(b) Perform a frequency calculation for reactants and products and compute the temperature $T_d$ at which the dehydrogenation becomes spontaneous.

(c) Compare your results with the analogous calculation of dehydrogenation $T_d$ for cyclopentane.

Solution Exercise 4: See tutorial notes on ab initio free energy calculations.

C. Moyses Araujo, Davide L. Simone, Steven J. Konezny, Aaron Shim, Robert H. Crabtree, Grigorii L. Soloveichik, and Victor S. Batista

\[ \text{LH}_n \leftrightarrow \text{L} + n\text{H}^+ + ne^- \]
\[ + \frac{n}{4} \text{O}_2 + n\text{H}^+ \leftrightarrow \frac{n}{2} \text{H}_2\text{O} - ne^- \]
\[ \text{LH}_n + \frac{n}{4} \text{O}_2 \leftrightarrow \text{L} + \frac{n}{2} \text{H}_2\text{O} \]

\[ E^0 = -\Delta G_r/nF \]
\[ \Delta G_r = G_L + \frac{n}{2} G_{\text{H}_2\text{O}} - G_{\text{LH}_n} - \frac{n}{4} G_{\text{O}_2} \]

\[ H = E_{\text{elect}} + U_{\text{vib}} + U_{\text{trans}} + U_{\text{rot}} + PV \]
\[ G = H - T(S_{\text{vib}} + S_{\text{rot}} + S_{\text{trans}}) \]
\[ H = H^0 + C_p(T - 298.15 \text{ K}) \]
\[ S = S^0 + C_p \ln(T/298.15 \text{ K}) \]

C. Moyses Araujo, Davide L. Simone, Steven J. Konezny, Aaron Shim, Robert H. Crabtree, Grigorii L. Soloveichik, and Victor S. Batista

Calculated open circuit potentials and hydrogen gravimetric densities for six- (type A) and five-member (type C) ring fuels.

<table>
<thead>
<tr>
<th>Name</th>
<th>Structure</th>
<th>H, wt. %</th>
<th>E⁰, V</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzene</td>
<td><img src="image1" alt="Benzene" /></td>
<td>7.19</td>
<td>1.049</td>
</tr>
<tr>
<td>Pyridine</td>
<td><img src="image2" alt="Pyridine" /></td>
<td>7.10</td>
<td>1.081</td>
</tr>
<tr>
<td>Pyrimidine</td>
<td><img src="image3" alt="Pyrimidine" /></td>
<td>7.02</td>
<td>1.116</td>
</tr>
<tr>
<td>Pyridazine</td>
<td><img src="image4" alt="Pyridazine" /></td>
<td>7.02</td>
<td>1.085</td>
</tr>
<tr>
<td>1,3,5-triazine</td>
<td><img src="image5" alt="1,3,5-triazine" /></td>
<td>6.94</td>
<td>1.198</td>
</tr>
<tr>
<td>Cyclopentadiene</td>
<td><img src="image6" alt="Cyclopentadiene" /></td>
<td>5.75</td>
<td>0.854</td>
</tr>
<tr>
<td>Furan</td>
<td><img src="image7" alt="Furan" /></td>
<td>5.59</td>
<td>1.004</td>
</tr>
<tr>
<td>1H-pyrrole</td>
<td><img src="image8" alt="1H-pyrrole" /></td>
<td>5.67</td>
<td>1.092</td>
</tr>
<tr>
<td>1H-imidazole</td>
<td><img src="image9" alt="1H-imidazole" /></td>
<td>5.59</td>
<td>1.203</td>
</tr>
<tr>
<td>1H-pyrazole</td>
<td><img src="image10" alt="1H-pyrazole" /></td>
<td>5.59</td>
<td>1.269</td>
</tr>
<tr>
<td>1H-1,2,3-triazole</td>
<td><img src="image11" alt="1H-1,2,3-triazole" /></td>
<td>5.52</td>
<td>1.351</td>
</tr>
<tr>
<td>1H-1,2,4-triazole</td>
<td><img src="image12" alt="1H-1,2,4-triazole" /></td>
<td>5.52</td>
<td>1.328</td>
</tr>
</tbody>
</table>

Correlation between OCP’s obtained from the calculated free energies at B3LYP/cc-PVTZ theory level and from the experimental thermodynamic data (NIST database).
C. Moyses Araujo, Davide L. Simone, Steven J. Konezny, Aaron Shim, Robert H. Crabtree, Grigorii L. Soloveichik, and Victor S. Batista

Calculated open circuit potentials and hydrogen gravimetric densities for fused six- (type D) and five-member (type E) ring fuels.

<table>
<thead>
<tr>
<th>Organic carrier (in dehydrogenated state)</th>
<th>H, wt. %</th>
<th>E', V</th>
</tr>
</thead>
<tbody>
<tr>
<td>1H-indene</td>
<td>6.49</td>
<td>1.041</td>
</tr>
<tr>
<td>benzofuran</td>
<td>6.39</td>
<td>1.084</td>
</tr>
<tr>
<td>benzo[5]thiophene</td>
<td>5.67</td>
<td>1.080</td>
</tr>
<tr>
<td>1H-indole</td>
<td>6.54</td>
<td>1.128</td>
</tr>
<tr>
<td>2H-isindole</td>
<td>6.54</td>
<td>1.092</td>
</tr>
<tr>
<td>indolizine</td>
<td>6.54</td>
<td>1.064</td>
</tr>
<tr>
<td>1H-indazole</td>
<td>6.49</td>
<td>1.206</td>
</tr>
<tr>
<td>1H-pyrmolo [2,3-b]pyridine</td>
<td>6.39</td>
<td>1.167</td>
</tr>
<tr>
<td>imidazo[1,2-a] pyrazine</td>
<td>6.34</td>
<td>1.145</td>
</tr>
<tr>
<td>7H-purine</td>
<td>6.29</td>
<td>1.228</td>
</tr>
<tr>
<td>1,4-dihydropentalene</td>
<td>5.49</td>
<td>0.901</td>
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<tr>
<td>1H-pyrmolozine</td>
<td>6.44</td>
<td>1.017</td>
</tr>
<tr>
<td>1,4-dihydropyrrole [3,2-b]pyrole</td>
<td>5.39</td>
<td>1.159</td>
</tr>
<tr>
<td>1,4-dihydropyrrole [4,5-d]imidazo</td>
<td>5.30</td>
<td>1.313</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Organic carrier (in dehydrogenated state)</th>
<th>H, wt. %</th>
<th>E', V</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>Structure</td>
<td></td>
</tr>
<tr>
<td>naphthalene</td>
<td><img src="image" alt="naphthalene" /></td>
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<td><img src="image" alt="quinoline" /></td>
<td>7.24</td>
</tr>
<tr>
<td>isoquinoline</td>
<td><img src="image" alt="isoquinoline" /></td>
<td>7.24</td>
</tr>
<tr>
<td>4H-quinolizine</td>
<td><img src="image" alt="4H-quinolizine" /></td>
<td>5.79</td>
</tr>
<tr>
<td>cinnoline</td>
<td><img src="image" alt="cinnoline" /></td>
<td>7.19</td>
</tr>
<tr>
<td>phthalazine</td>
<td><img src="image" alt="phthalazine" /></td>
<td>7.19</td>
</tr>
<tr>
<td>quinazoline</td>
<td><img src="image" alt="quinazoline" /></td>
<td>7.19</td>
</tr>
<tr>
<td>quinoxaline</td>
<td><img src="image" alt="quinoxaline" /></td>
<td>7.19</td>
</tr>
<tr>
<td>1,8-naphthryidine</td>
<td><img src="image" alt="1,8-naphthryidine" /></td>
<td>7.19</td>
</tr>
<tr>
<td>1,5-naphthryidine</td>
<td><img src="image" alt="1,5-naphthryidine" /></td>
<td>7.19</td>
</tr>
<tr>
<td>pteridine</td>
<td><img src="image" alt="pteridine" /></td>
<td>7.09</td>
</tr>
<tr>
<td>pyrazino[2,3-b]pyrazine</td>
<td><img src="image" alt="pyrazino[2,3-b]pyrazine" /></td>
<td>7.09</td>
</tr>
<tr>
<td>pyrmido[4,5-d]pyrimidine</td>
<td><img src="image" alt="pyrmido[4,5-d]pyrimidine" /></td>
<td>7.09</td>
</tr>
</tbody>
</table>
C. Moyses Araujo, Davide L. Simone, Steven J. Konezny, Aaron Shim, Robert H. Crabtree, Grigorii L. Soloveichik, and Victor S. Batista

Boiling point, specific energy and energy density of selected organic fuels, and theoretical efficiency of fuel cells based on dehydrogenation.

<table>
<thead>
<tr>
<th>Organic carrier (in dehydrogenated state)</th>
<th>H, wt %</th>
<th>$E^0$, V</th>
</tr>
</thead>
<tbody>
<tr>
<td>9H-fluorene</td>
<td>6.78</td>
<td>1.109</td>
</tr>
<tr>
<td>dibenzo[1,2-b:3,4-b']furan</td>
<td>6.71</td>
<td>1.125</td>
</tr>
<tr>
<td>dibenzo[1,2-b:3,4-b']thiophene</td>
<td>6.16</td>
<td>1.117</td>
</tr>
<tr>
<td>5H-dibenzo[1,2-b:3,4-b']borole</td>
<td>6.81</td>
<td>1.108</td>
</tr>
<tr>
<td>9H-carbazole</td>
<td>6.75</td>
<td>1.152</td>
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<tr>
<td>9H-pyrollo [2,3-b:5,4-b']dipyridine</td>
<td>6.67</td>
<td>1.206</td>
</tr>
<tr>
<td>5H-pyrollo [3,2-c:4,5-c']dipyridine</td>
<td>6.67</td>
<td>1.191</td>
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<tr>
<td>5H-pyrollo [3,2-b:4,5-b']dipyridine</td>
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<td>1.181</td>
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<td>9X-carbazole</td>
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<td>1.152</td>
</tr>
<tr>
<td></td>
<td>Et</td>
<td>1.167</td>
</tr>
<tr>
<td>9X-1,8-diazacarbazole</td>
<td>H 6.67</td>
<td>1.206</td>
</tr>
<tr>
<td></td>
<td>Me</td>
<td>1.222</td>
</tr>
<tr>
<td></td>
<td>Et</td>
<td>1.230</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Organic carrier (in hydrogenated state)</th>
<th>Boiling point, °C</th>
<th>Specific energy, Wh/kg</th>
<th>Energy density, Wh/L</th>
<th>Efficiency, %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid hydrogen</td>
<td>-252.9</td>
<td>-</td>
<td>2539</td>
<td>83.0</td>
</tr>
<tr>
<td>Pyrrolidine</td>
<td>87</td>
<td>1660</td>
<td>1438</td>
<td>92.8</td>
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<tr>
<td>Tetrahydrofurane</td>
<td>66</td>
<td>1500</td>
<td>1334</td>
<td>93.4</td>
</tr>
<tr>
<td>Tetrahydrothiophene</td>
<td>119</td>
<td>1196</td>
<td>1195</td>
<td>93.5</td>
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<tr>
<td>Cyclohexane</td>
<td>80.7</td>
<td>2025</td>
<td>1578</td>
<td>94.1</td>
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<tr>
<td>Methylcyclohexane</td>
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<td>1747</td>
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<tr>
<td>Cyclohexylamine</td>
<td>134.5</td>
<td>1772</td>
<td>1532</td>
<td>95.2</td>
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<tr>
<td>Chlorocyclohexane</td>
<td>66</td>
<td>1403</td>
<td>1403</td>
<td>93.4</td>
</tr>
<tr>
<td>Cyclohexanol</td>
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<td>1686</td>
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<td>93.0</td>
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<tr>
<td>Cyclohexanethiol</td>
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<td>94.0</td>
</tr>
<tr>
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<td>2046</td>
<td>1764</td>
<td>94.2</td>
</tr>
<tr>
<td>2-methylpiperidine</td>
<td>118</td>
<td>1776</td>
<td>1499</td>
<td>94.5</td>
</tr>
<tr>
<td>Piperazine</td>
<td>146</td>
<td>2055</td>
<td>2260</td>
<td>95.7</td>
</tr>
<tr>
<td>trans-Decalin</td>
<td>187</td>
<td>2095</td>
<td>1877</td>
<td>93.1</td>
</tr>
</tbody>
</table>
Modeling Systems for CO₂/CO Conversion

Lesson From CO Dehydrogenases
Modeling Systems for CO/CO₂ Conversion

**Crabtree’s Biomimetic Ni Catalyst**

\[ \text{CO} + \text{H}_2\text{O} + 2\text{AcO}^- + 2\text{mv}^{2+} \rightleftharpoons \text{CO}_2 + 2\text{AcOH} + 2\text{mv}^+ \]

Inverse Design of Electrocatalysts: CO/CO\textsubscript{2} Conversion

Crabtree’s Biomimetic Ni Catalyst

Dr. Dequan Xiao
Dr. Ingolf Warnke

DFT Catalytic Cycle

1 \([\text{Ni}^{II}(\text{H}_2\text{O})]^0\)

2 \([\text{Ni}^{III}(\text{CO})](\text{H}_2\text{O})]^0\)

3 \([\text{Ni}^{III}(\text{COOH})]\)

4 \([\text{Ni}^{III}(\text{COOH})(\text{H}_2\text{O})]^0\)

4' \([\text{Ni}^{III}(\text{COO})]^2-\)

5 \([\text{Ni}^{III}(\text{CO}_2)(\text{H}_2\text{O})]^+\)

Solvent Displacement

Carboxylic Formation

PCET

\(\text{H}^+\)

\(\text{H}_2\text{O}\)

\(\text{CO}\)

\(\text{e}^-+\text{CO}_2\)
Free Energy (kcal/mol)

-20
-15
-10
-5
0
5
10
15

Reaction Coordinate

1: [LNi^{III}(H_2O)]^0
2: [LNi^{II}(CO)]^0
3: [LNi^{II}(COOH)]^-
4: [LNi^{III}(COOH)(H_2O)]^0
5: [LNi^{I}(CO_2)(H_2O)]^-

Dimer

-11.4
-4.2
-0.6
-1.9
+1.1
-0.1
+4.8
+8.1
-16.0
-11.2

CO_2 + 34 kcal/mol

Original cycle (black)
ID optimized (red)

Aldrich 1?
The Fischer-Tropsch Process

1) Synthesis Gas Formation

\[ \text{CH}_n + \text{O}_2 \xrightarrow{\text{(Catalyst)}} \frac{1}{2} n \text{H}_2 + \text{CO} \]

2) Fischer-Tropsch Reaction

\[ 2n \text{H}_2 + \text{CO} \xrightarrow{\text{Catalyst}} -(\text{CH}_2^-)_n^- + \text{H}_2\text{O} \]

3) Refining

\[ -(\text{CH}_2^-)_n^- \xrightarrow{\text{(Catalyst)}} \text{Fuels, lubricants, etc.} \]
Modeling Systems for CO$_2$ Conversion

Lesson From Rubisco: CC Bond Formation

Natural CO$_2$ Fixation based on Mg Catalysts?

Carboxylation in Ribulose 1,5-BisPhosphate carboxylase (Rubisco)

$10^{11}$ metric tons of CO$_2$ per year are converted to organic material by the world’s most abundant enzyme.
Modeling Systems for CO$_2$ Conversion

Lesson From Rubisco: CC Bond Formation

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