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Computational Investigation of the Mechanism of an Octahedral Ni(II) Proton Reduction Catalyst and Importance of Intramolecular Hydrogen Bonding

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Bhattacharjee, Avik; Brown, Dayalis S.V.; Virca, Carolyn N.; Ethridge, Trent E.; Mendez Galue, Oreana; Pham, Uyen T.; and McCormick, Theresa M., "Computational Investigation of the Mechanism of an Octahedral Ni(II) Proton Reduction Catalyst and Importance of Intramolecular Hydrogen Bonding" (2022). *Student Research Symposium*. 15.

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Presenter Information

Avik Bhattacharjee, Dayalis S.V. Brown, Carolyn N. Virca, Trent E. Ethridge, Oreana Mendez Galue, Uyen T. Pham, and Theresa M. McCormick

Computational investigation of the mechanism of an octahedral Ni(II) proton reduction catalyst and importance of intramolecular hydrogen bonding

Avik Bhattacharjee

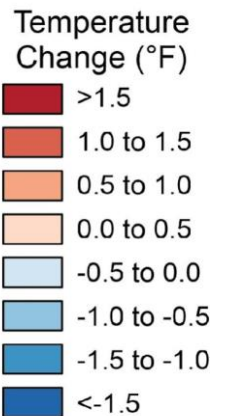
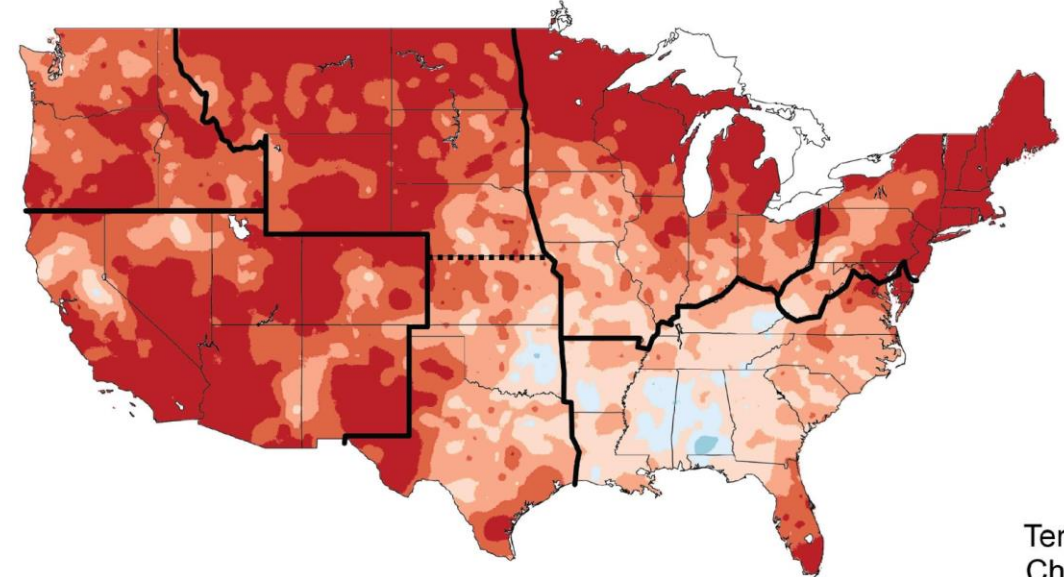
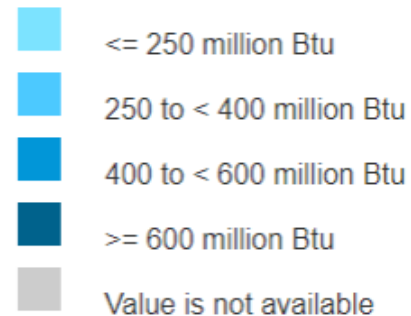
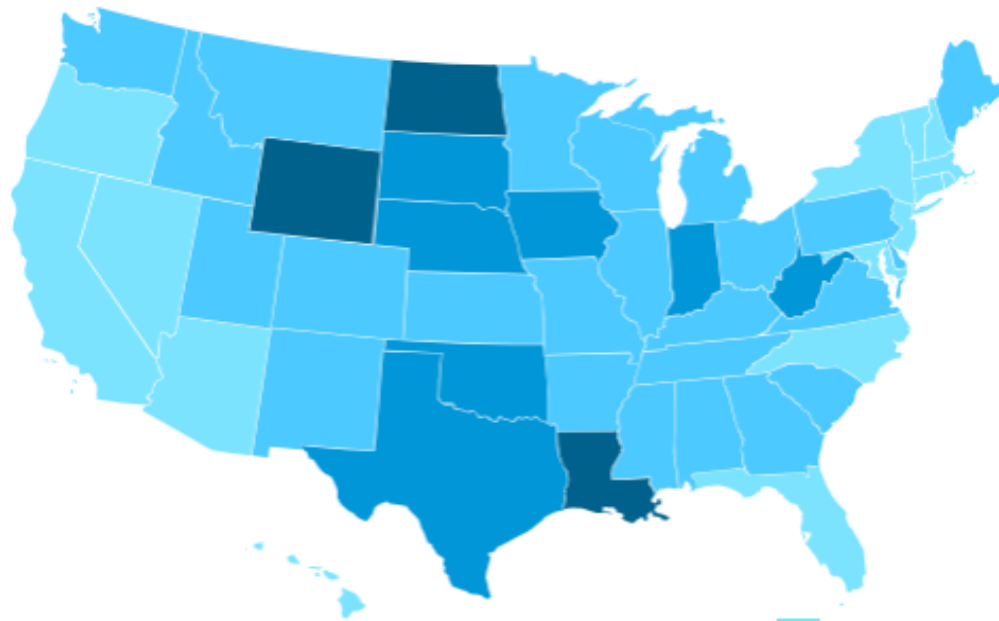
McCormick Group

Oral presentation

Student Research Symposium

05/04/2022

Use of fossil fuel and Climate Change



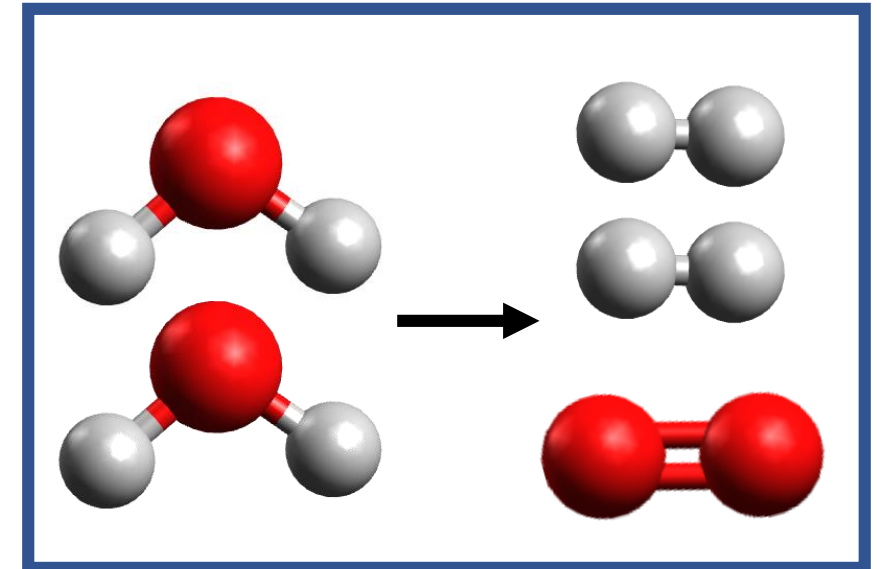
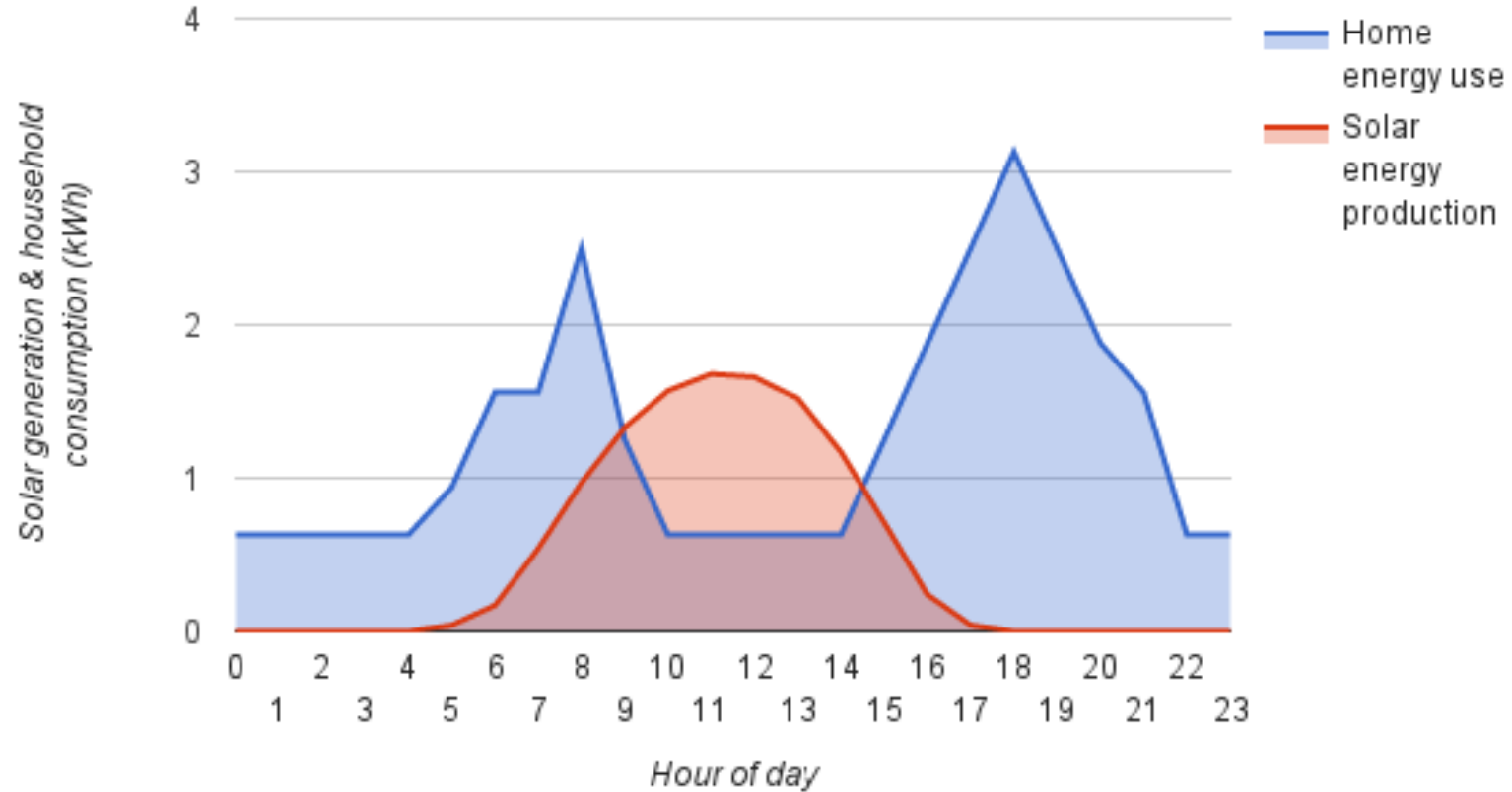
World Energy Council Congress – Enerdata ([Global energy Statistical Yearbook 2019](https://www.enerdata.net/global-energy-statistical-yearbook-2019/))

United States Energy Information Administration (eia.gov/state/rankings/)

United States Environmental protection Agency (<https://www.epa.gov/ghgemissions/sources-greenhouse-gas-emissions>)

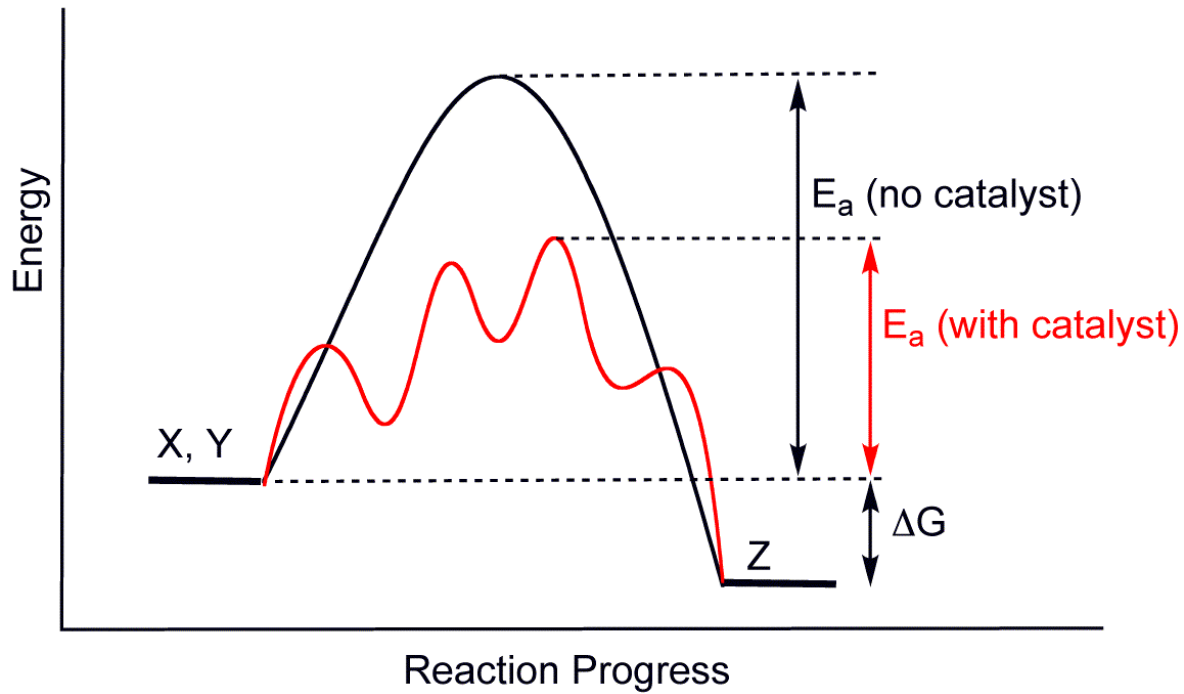
Climate changes in the United States: NASA earth observatory (<https://earthobservatory.nasa.gov/images/83624/climate-changes-in-the-united-states>)

Solar energy use and practical challenges

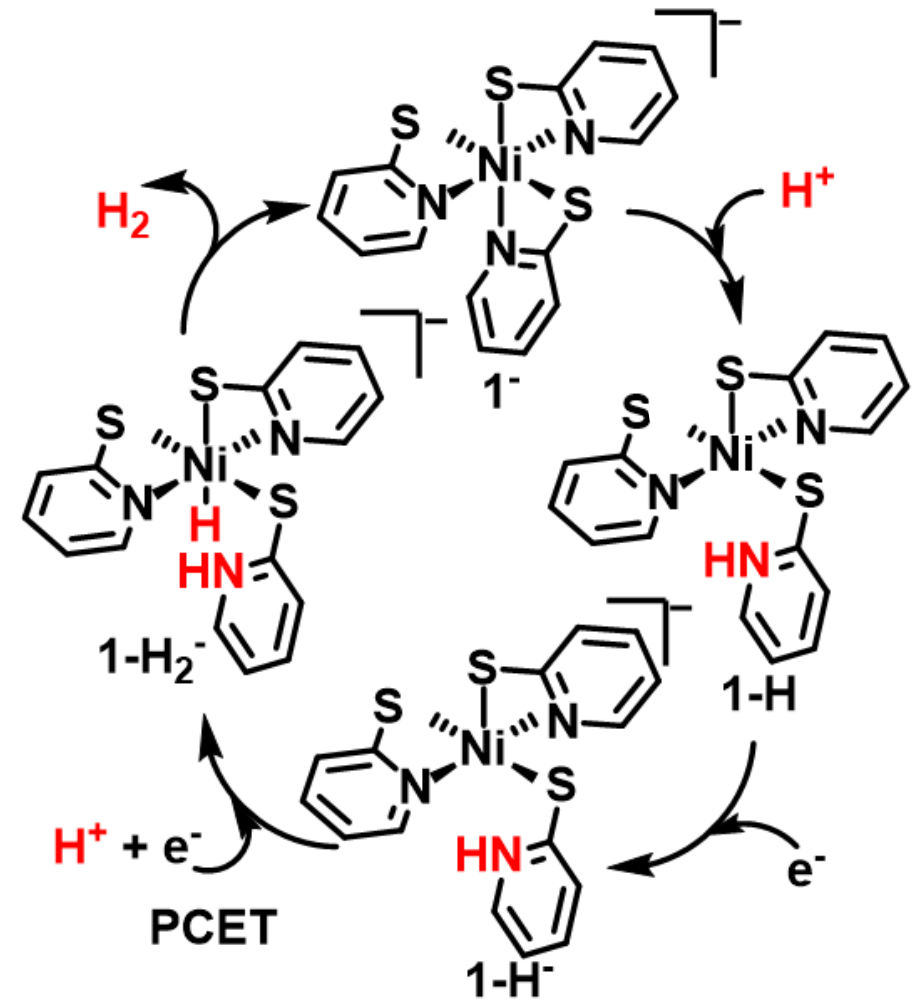


<https://www.solarchoice.net.au/blog/solar-self-consumption-overview/>

Catalysis and hydrogen production

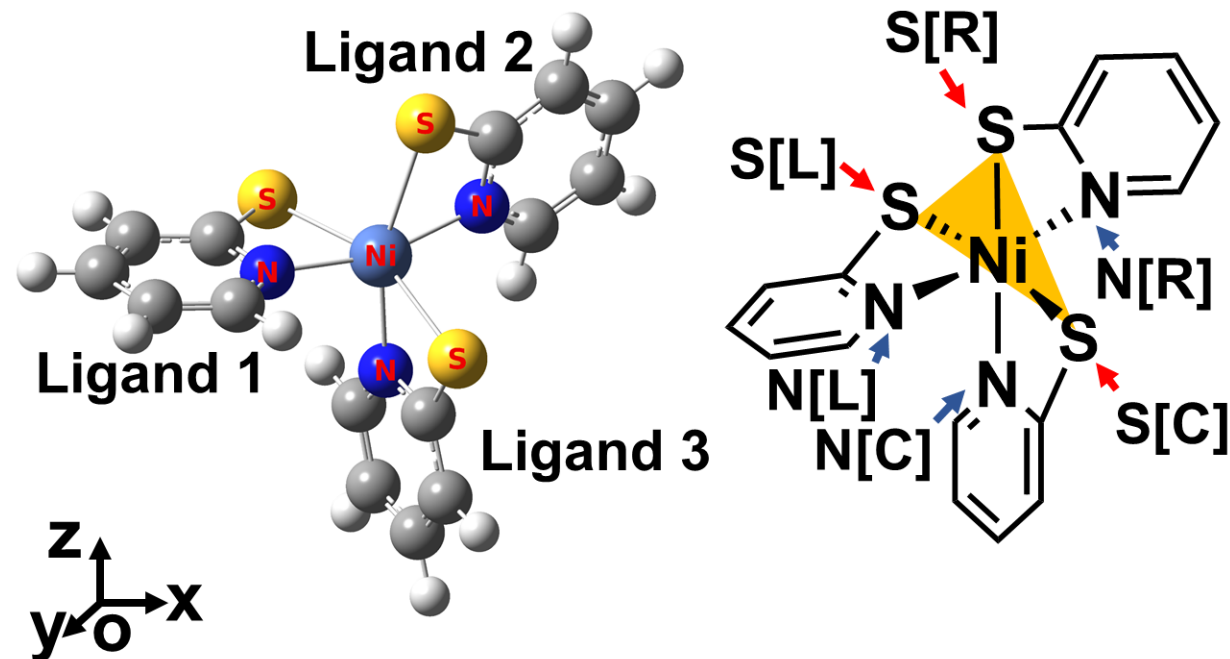
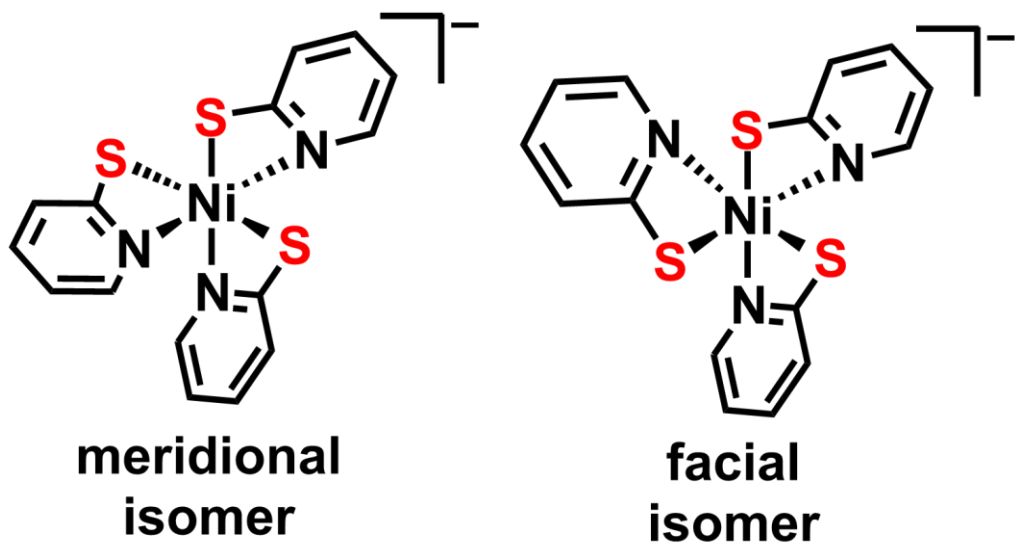


<https://en.wikipedia.org/wiki/Catalysis#/media/File:CatalysisScheme.png>

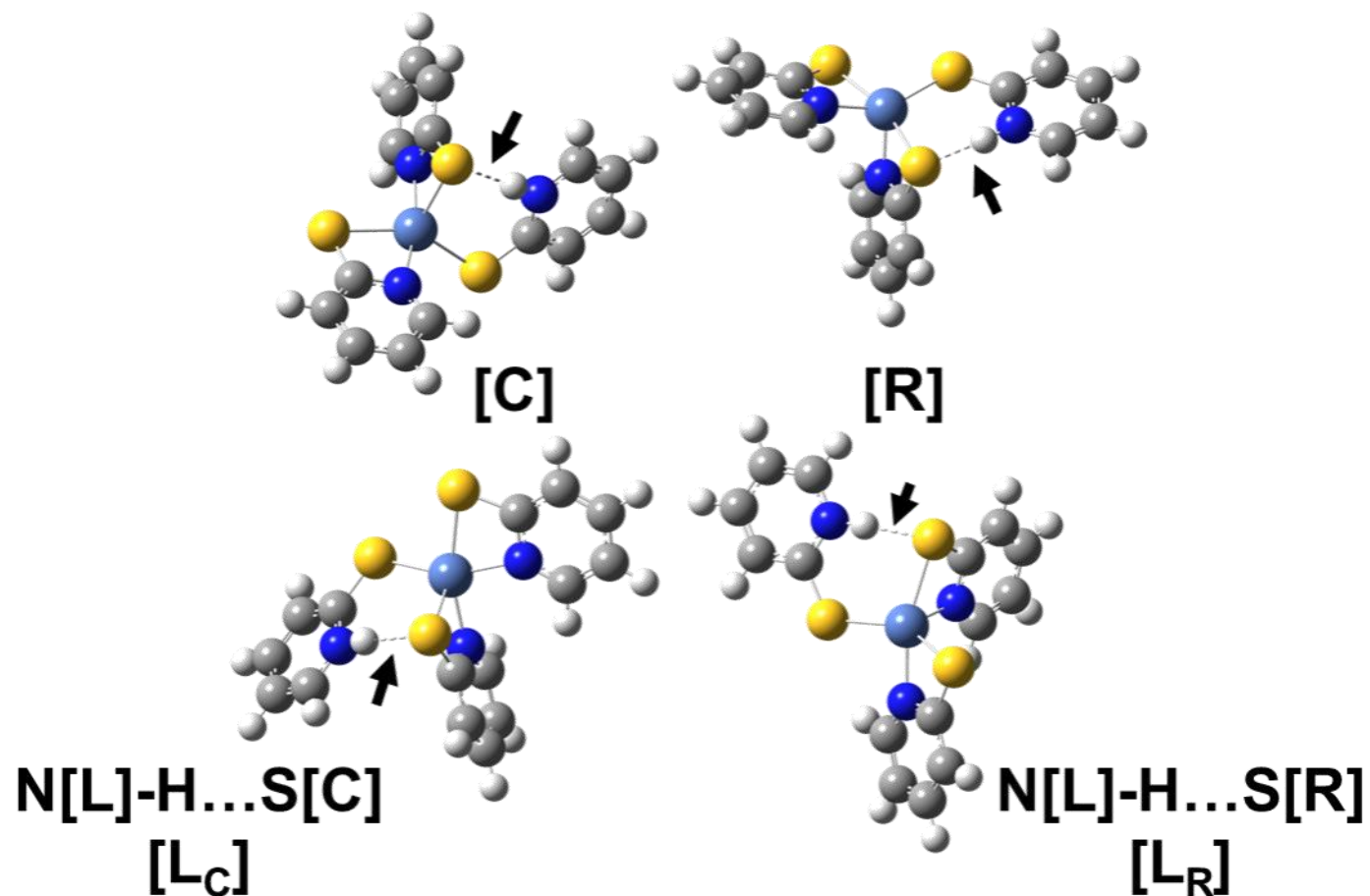
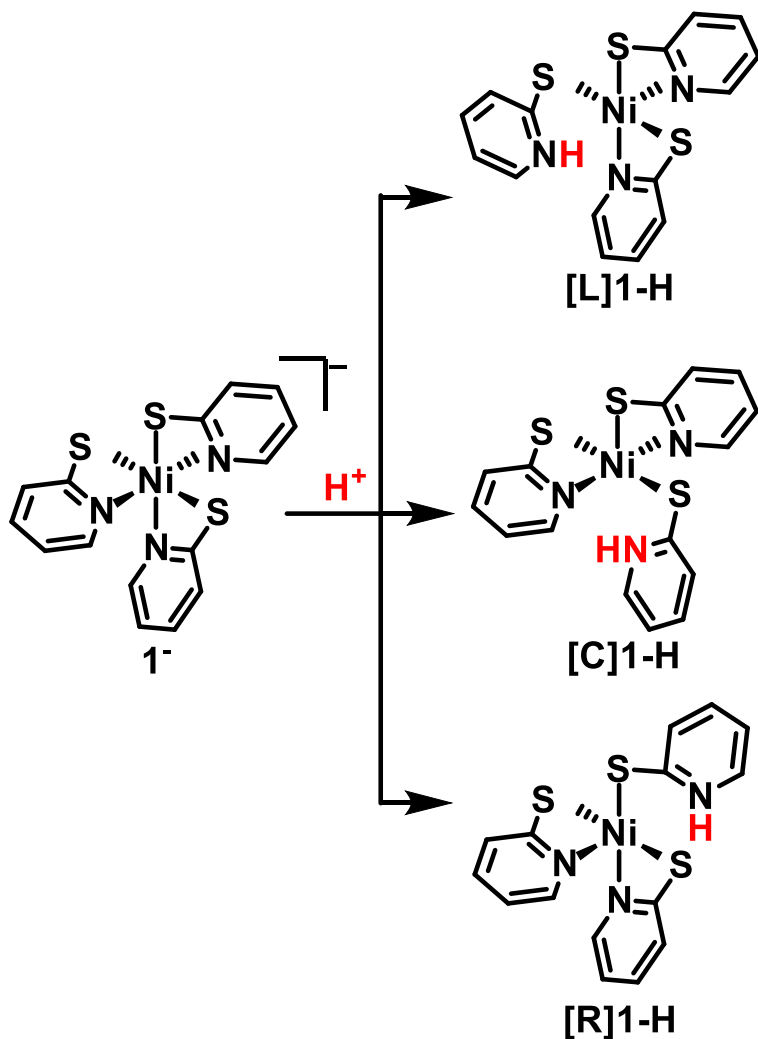


Dalton Trans. **2015**, *44*, 14333–14340.

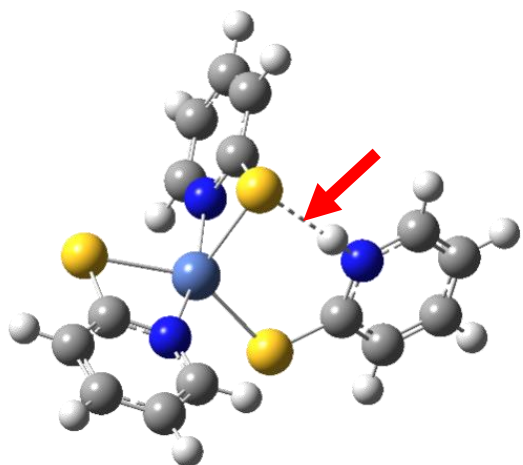
Structure and isomers of Ni(II) catalyst



Protonation of Ni(II) catalyst: *Expectation v. Reality*



Difference in isomer stability and property

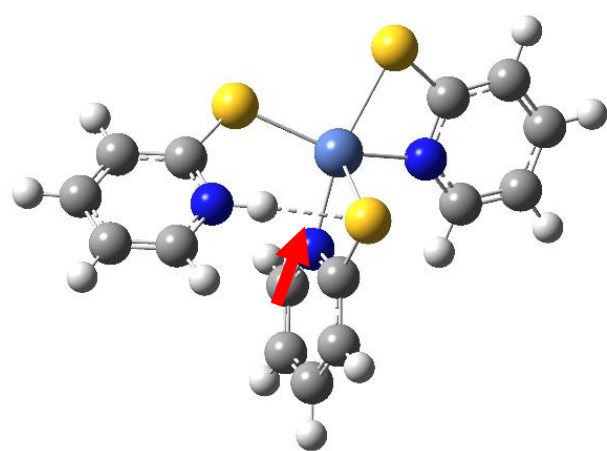


[C]

$pK_a = 11.4$

$\%x = 5.27$

$E^{HB} = -6.32$ kcal/mol



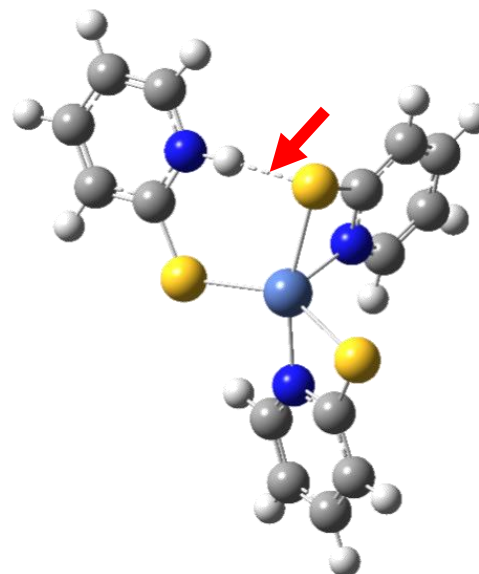
N[L]-H...S[C]

[L_C]

$pK_a = 11.1$

$\%x = 2.51$

$E^{HB} = -5.99$ kcal/mol



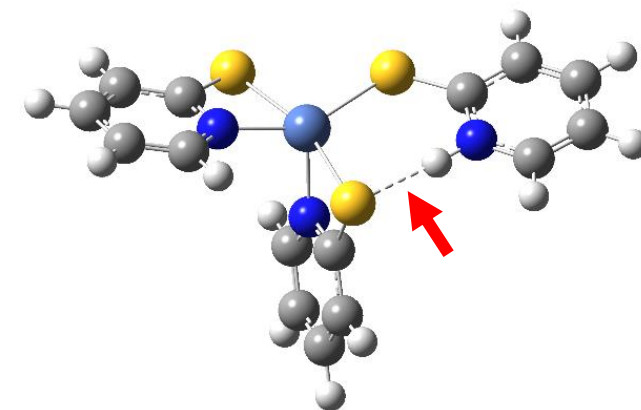
N[L]-H...S[R]

[L_R]

$pK_a = 12.2$

$\%x = 31.93$

$E^{HB} = -7.36$ kcal/mol



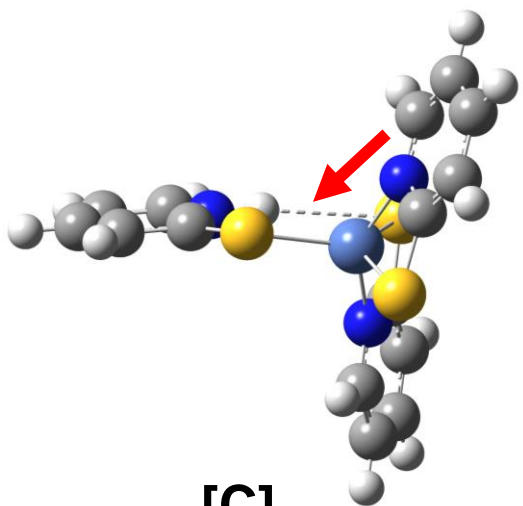
[R]

$pK_a = 12.4$

$\%x = 60.30$

$E^{HB} = -7.39$ kcal/mol

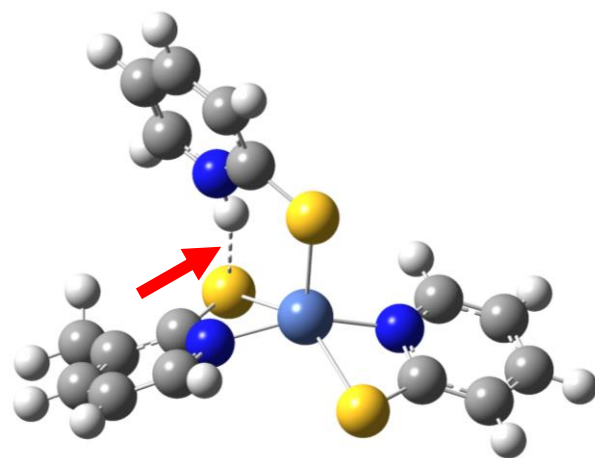
Reduction step of the catalysis



[C]

$\%x = 44.29$

$E^{\text{HB}} = -6.06 \text{ kcal/mol}$

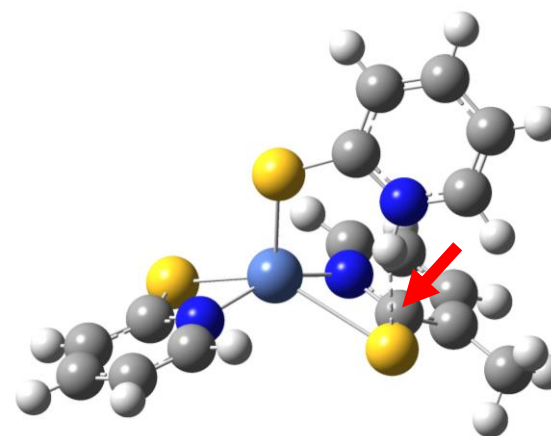


N[L]-H...S[C]

[L_C]

$\%x = 8.39$

$E^{\text{HB}} = -6.39 \text{ kcal/mol}$

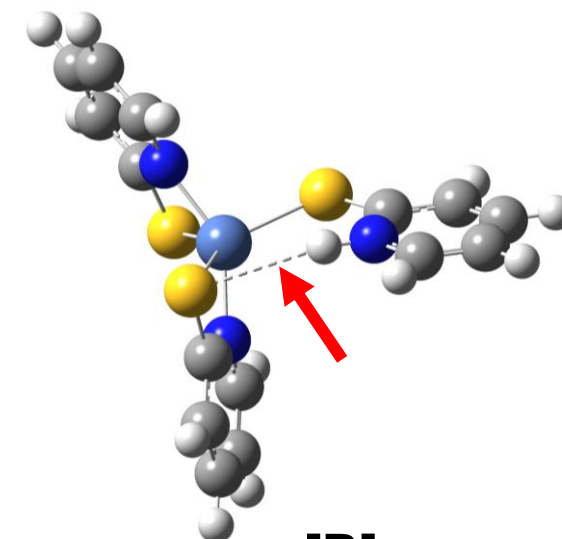


N[L]-H...S[R]

[L_R]

$\%x = 3.72$

$E^{\text{HB}} = -6.49 \text{ kcal/mol}$

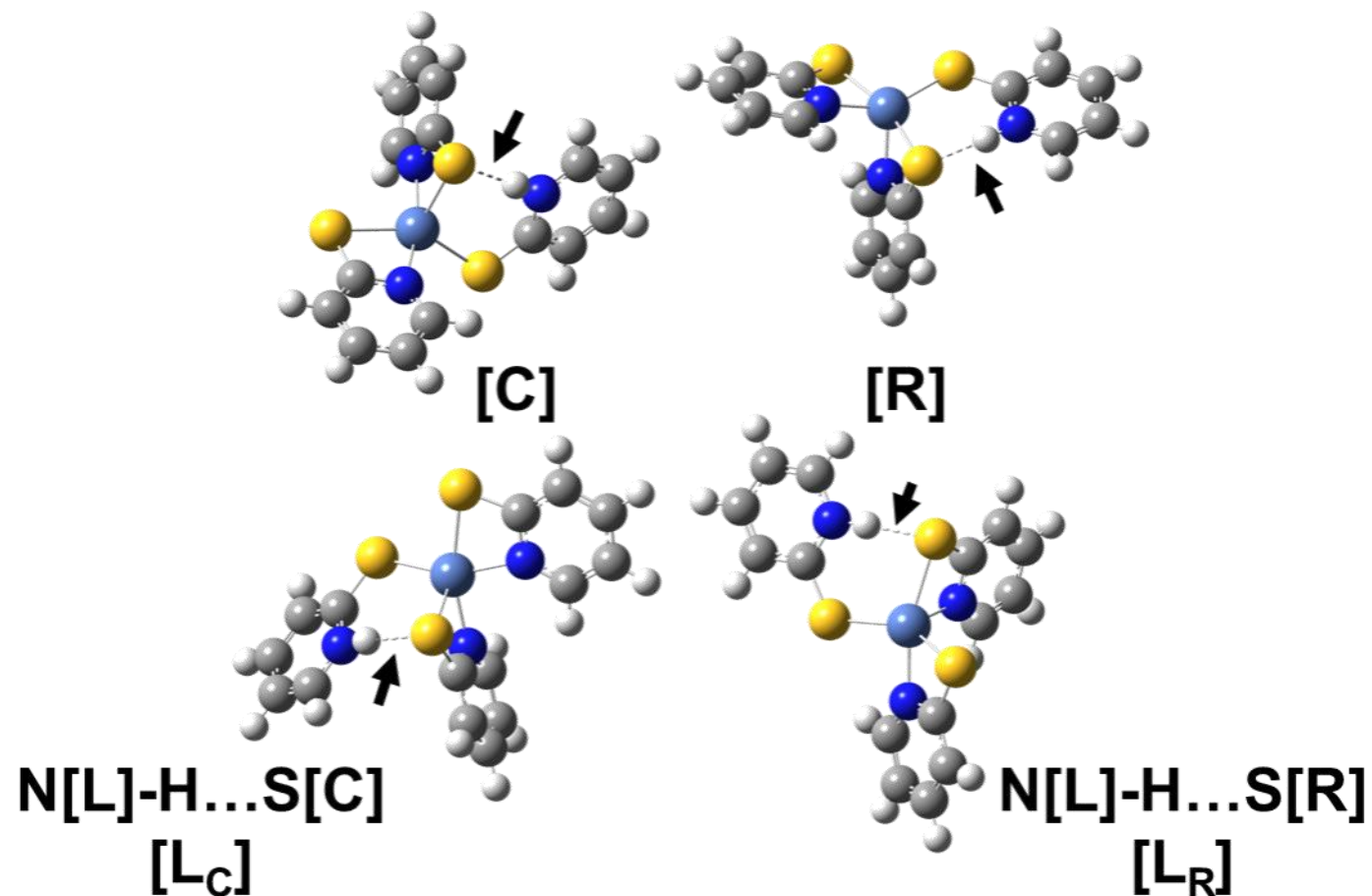
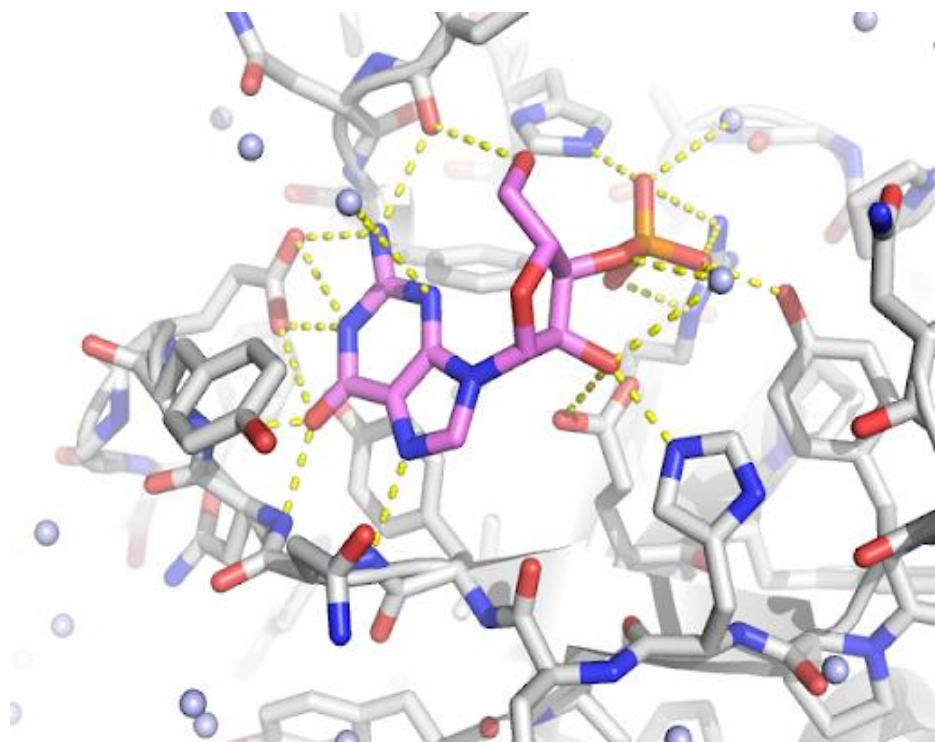


[R]

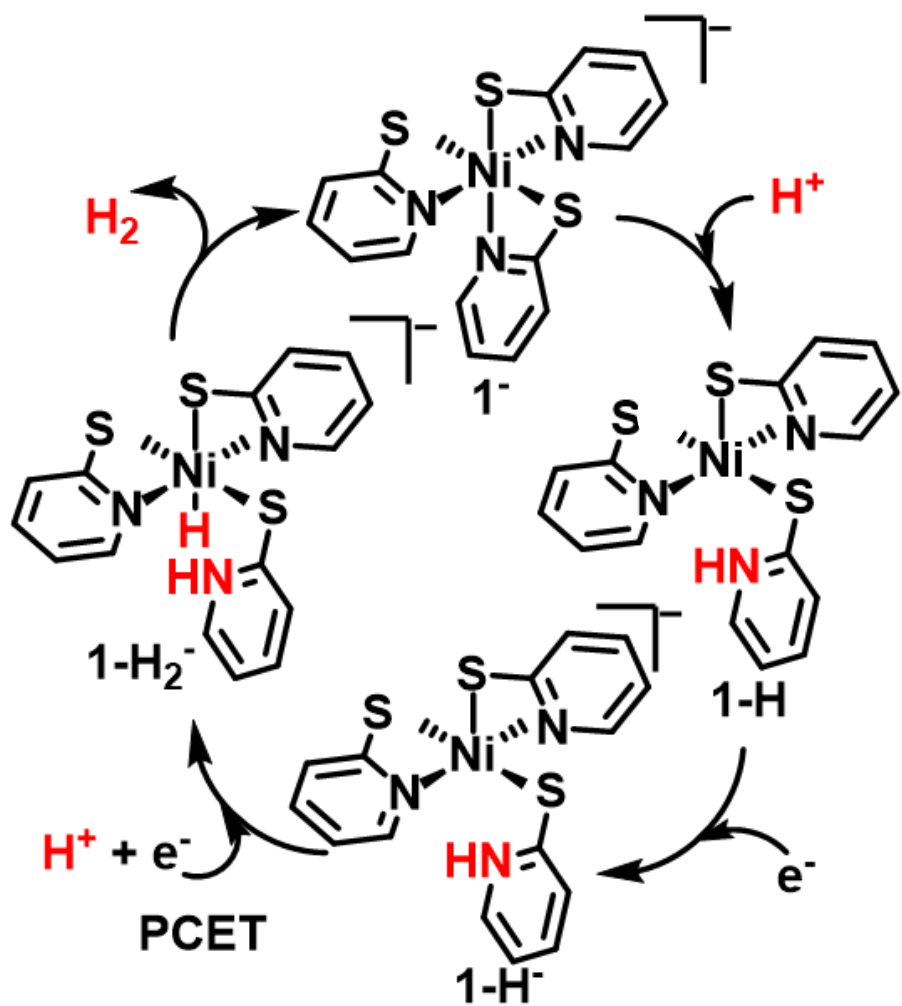
$\%x = 43.59$

$E^{\text{HB}} = -6.06 \text{ kcal/mol}$

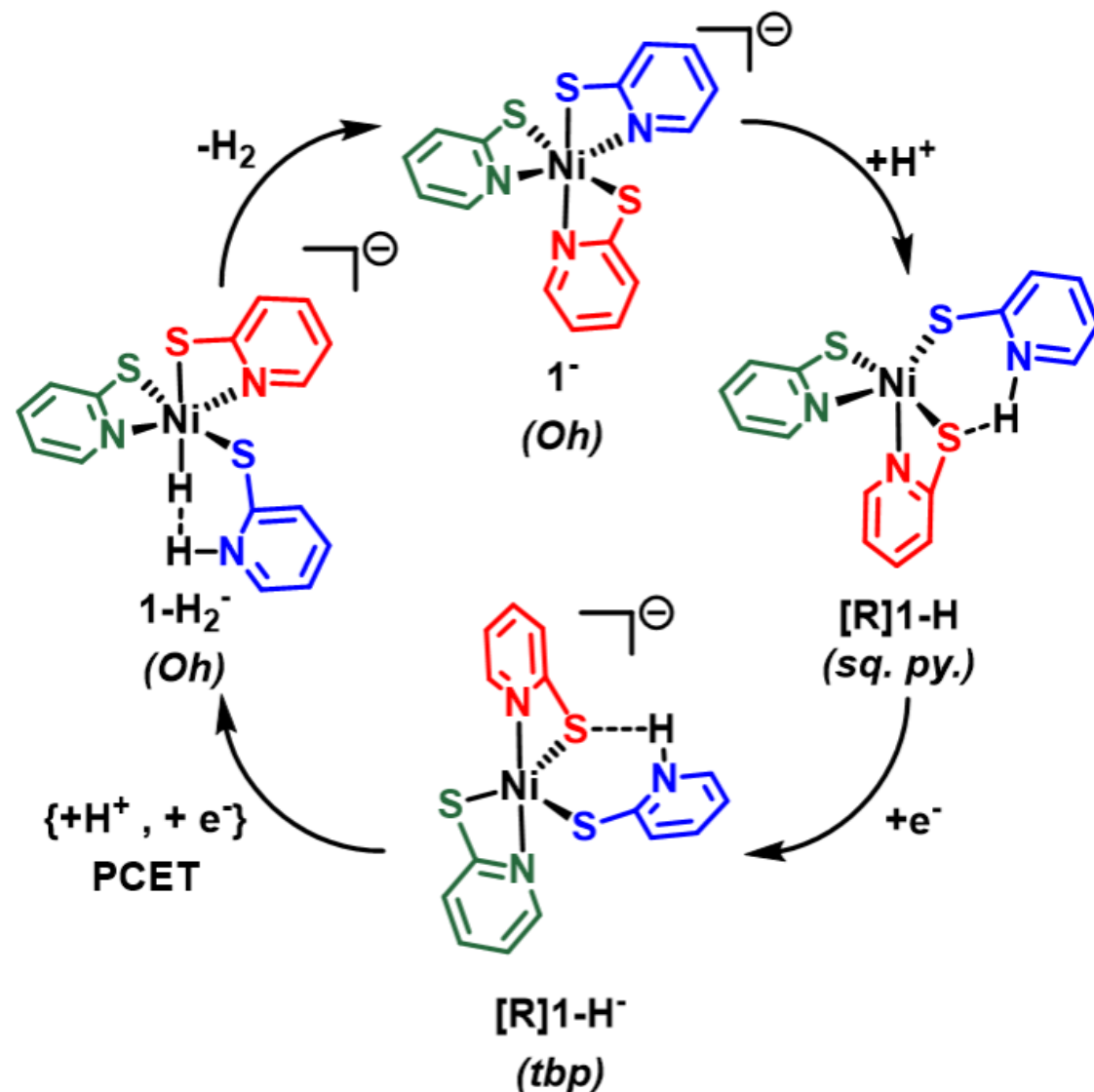
Importance of intramolecular H-bonding in small molecules



Effect of H-bonding on the catalytic cycle



Dalton Trans., **2015**, *44*, 14333-14340



Dalton Trans., **2022**, *51*, 3676-3685

Thank you

Dr. Theresa McCormick
Dayalis S. V. Brown
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Uyen Pham
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Dr. Luke Lutkus
Dr. Austin Shigemoto
Dr. Carolyn Virca
Prof. Eric Rivard
Dr. Kodi Beyeh
Dr. David Stuart

