May 4th, 9:00 AM - 11:00 AM

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

Avik Bhattacharjee
Portland State University

Dayalis S.V. Brown
Portland State University

Carolyn N. Virca
Portland State University

Trent E. Ethridge
Portland State University

Oreana Mendez Galue
Portland State University

Presenter Information

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

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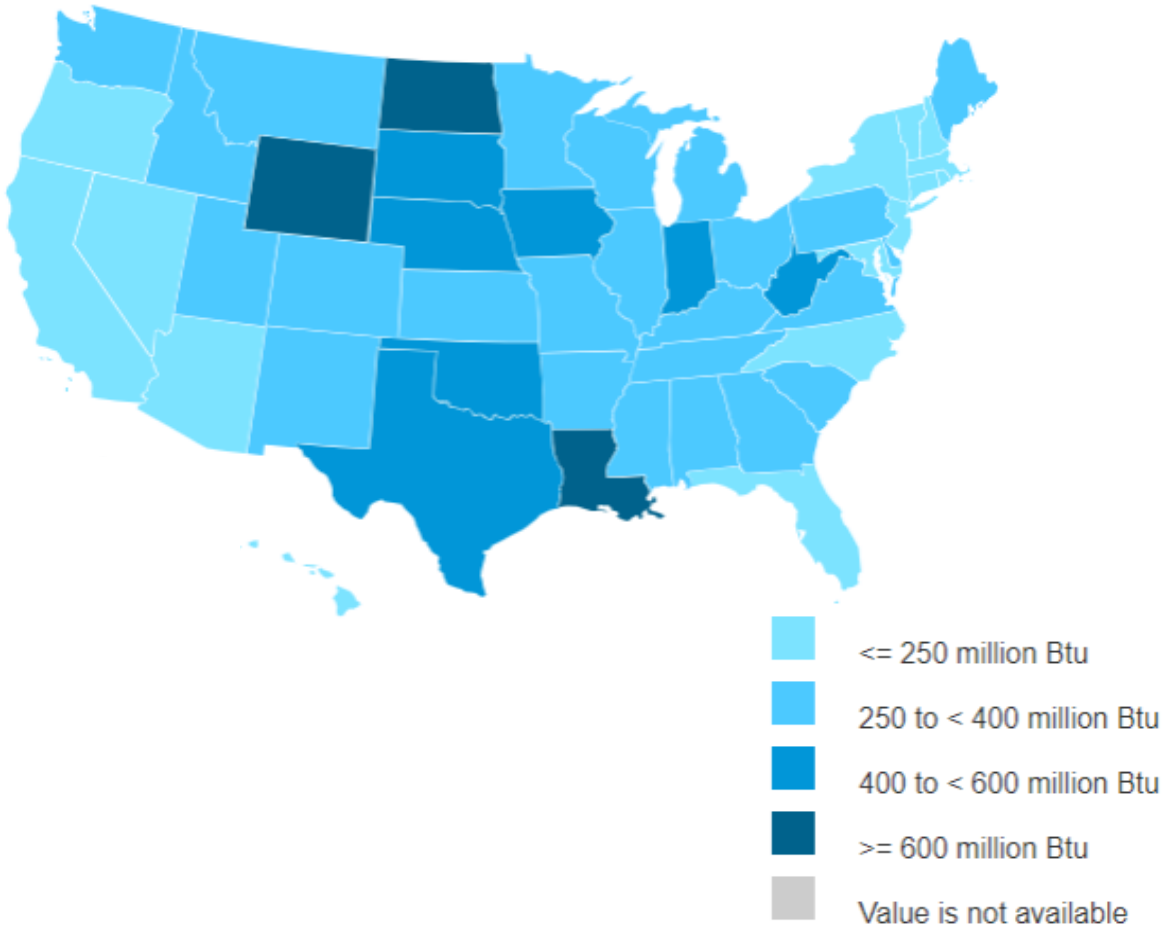
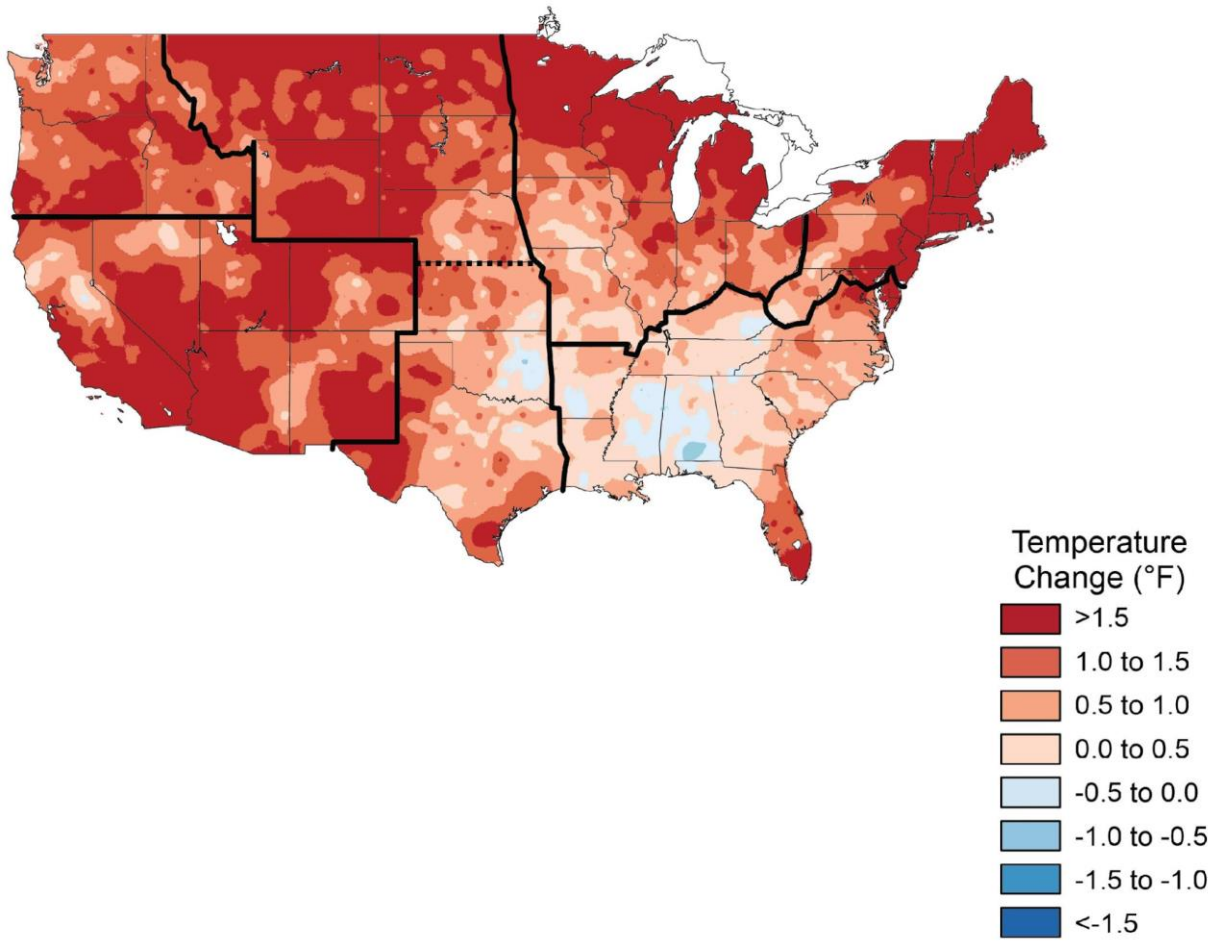
Avik Bhattacharjee
McCormick Group
Oral presentation
Student Research Symposium
05/04/2022

Portland State
UNIVERSITY

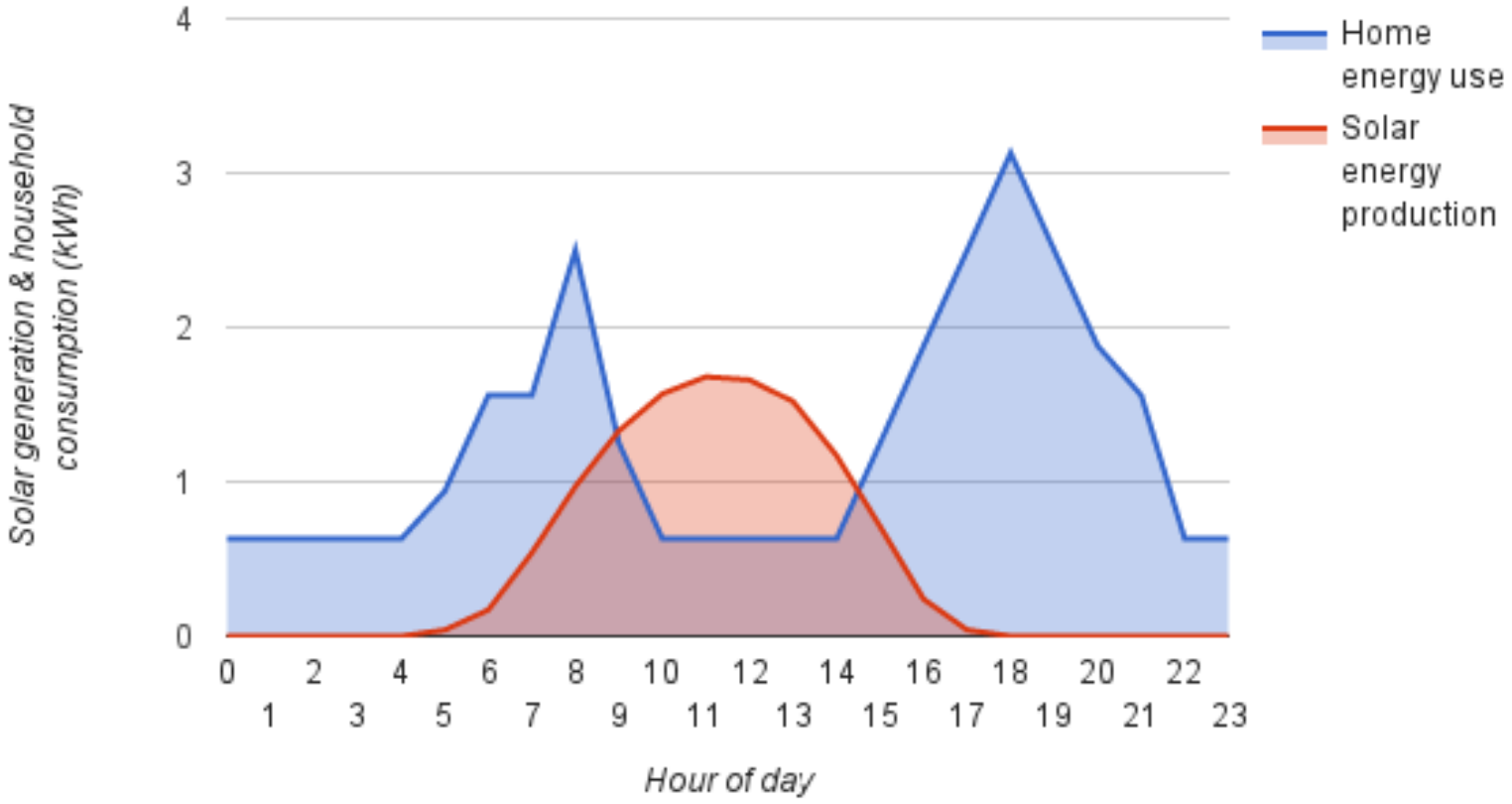
Use of fossil fuel and Climate Change

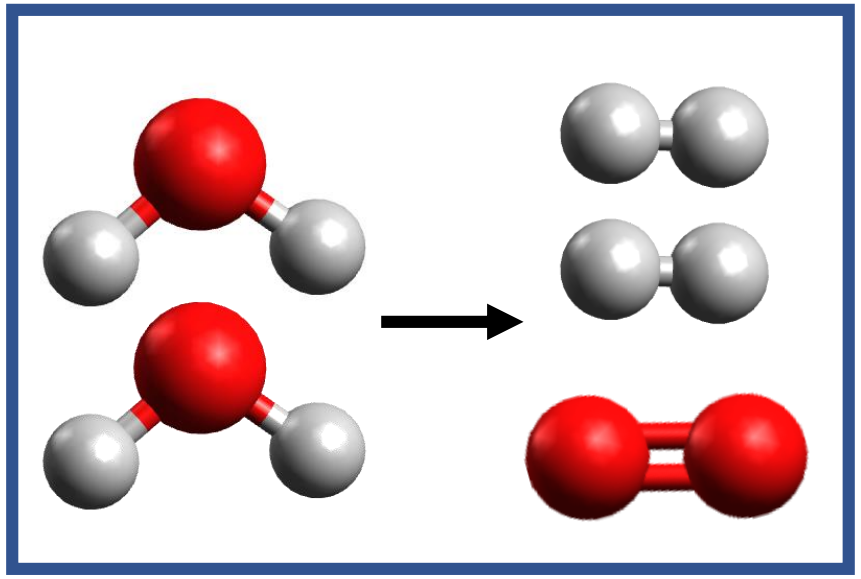




World Energy Council Congress – Enerdata (Global energy Statistical Yearbook 2019)
United States Energy Information Administration (eia.gov/state/rankings/)
United States Environmental protection Agency (https://www.epa.gov/ghgemissions/sources-greenhouse-gas-emissions)
Climate changes in the United States: NASA earth observatory (https://earthobservatory.nasa.gov/images/83624/climate-changes-in-the-united-states

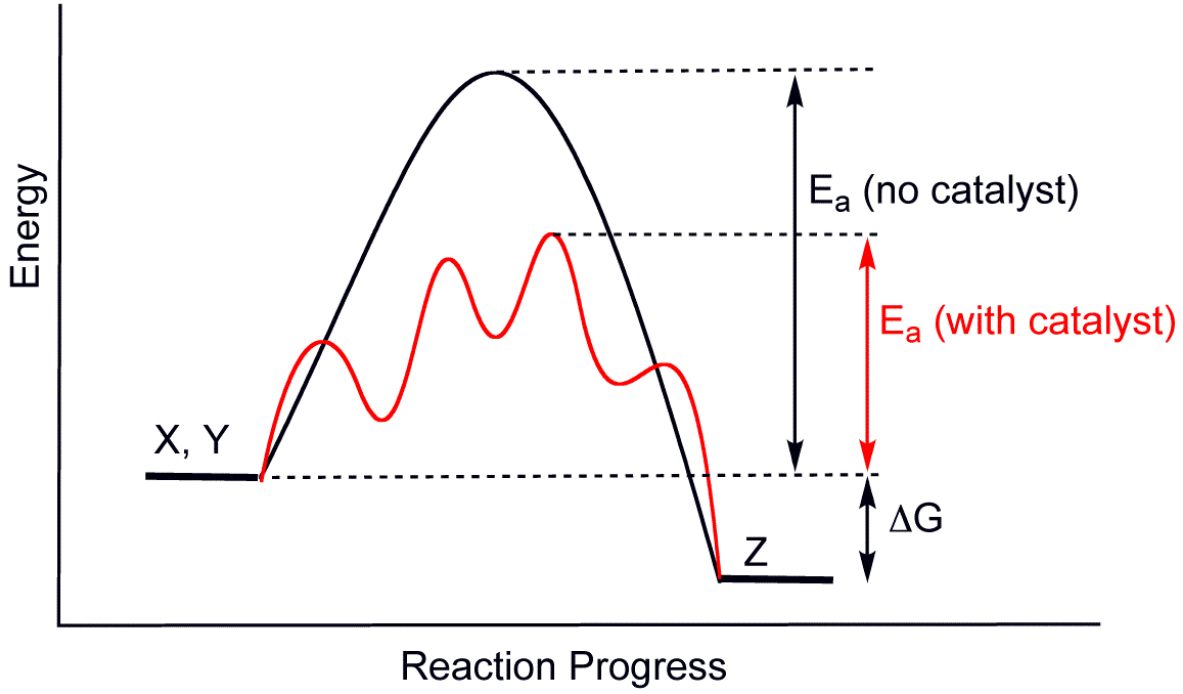
Solar energy use and practical challenges



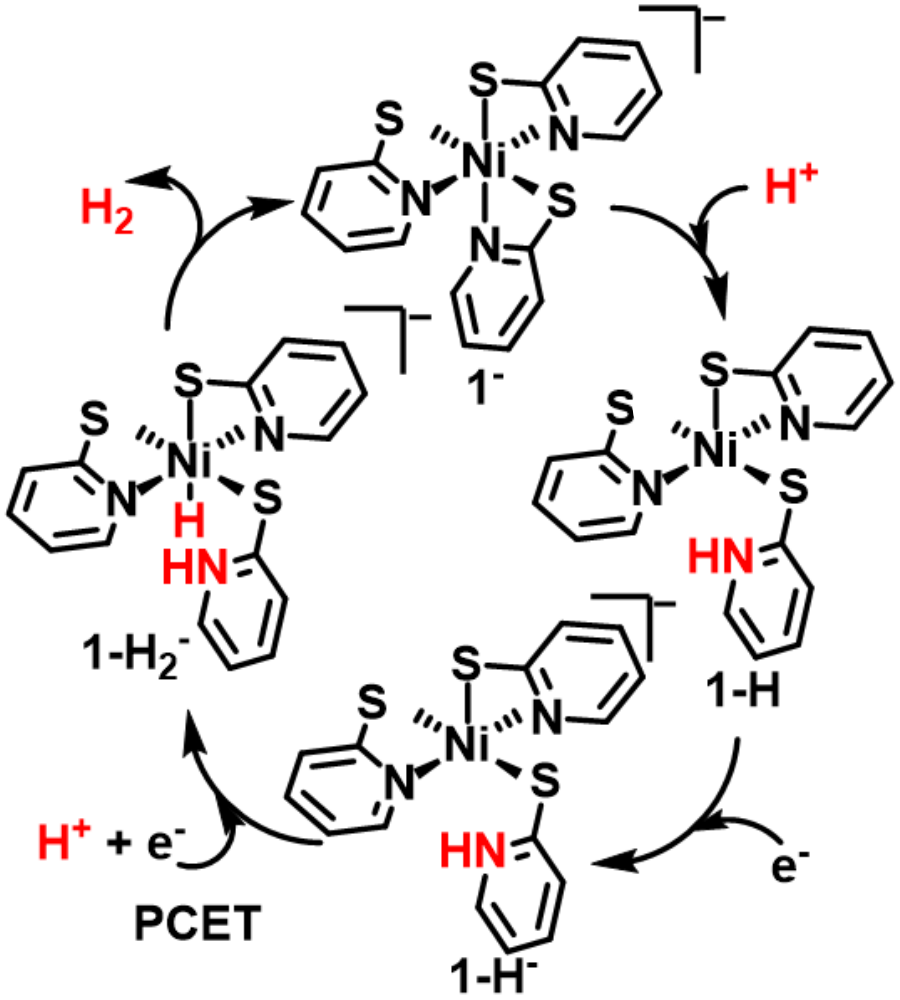


https://www.solarchoice.net.au/blog/solar-self-consumption-overview/

Catalysis and hydrogen production



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



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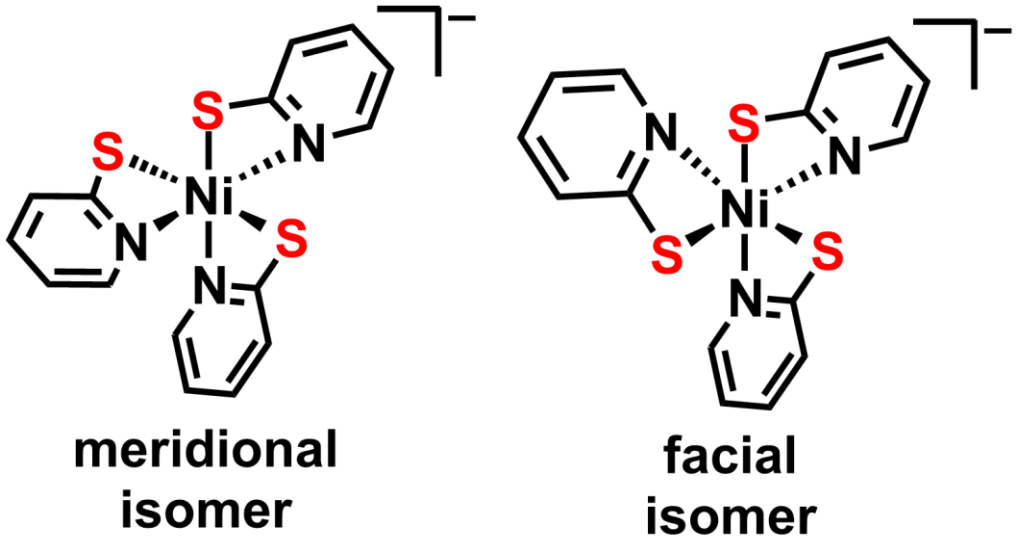
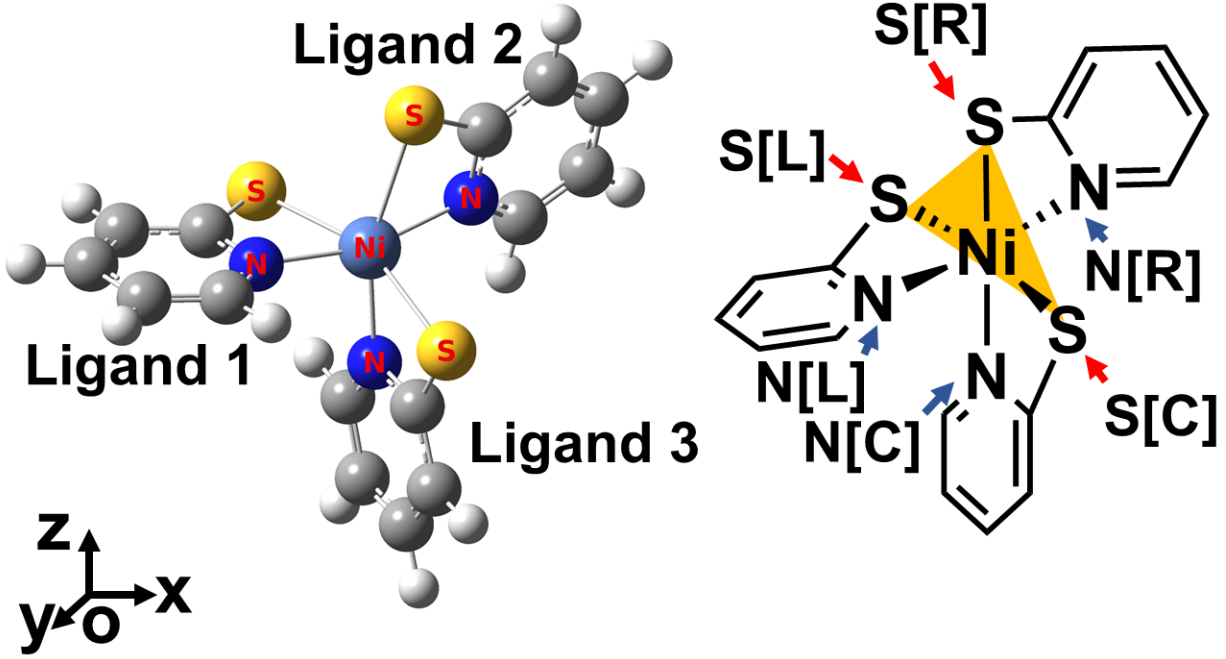
Structure and isomers of Ni(II) catalyst





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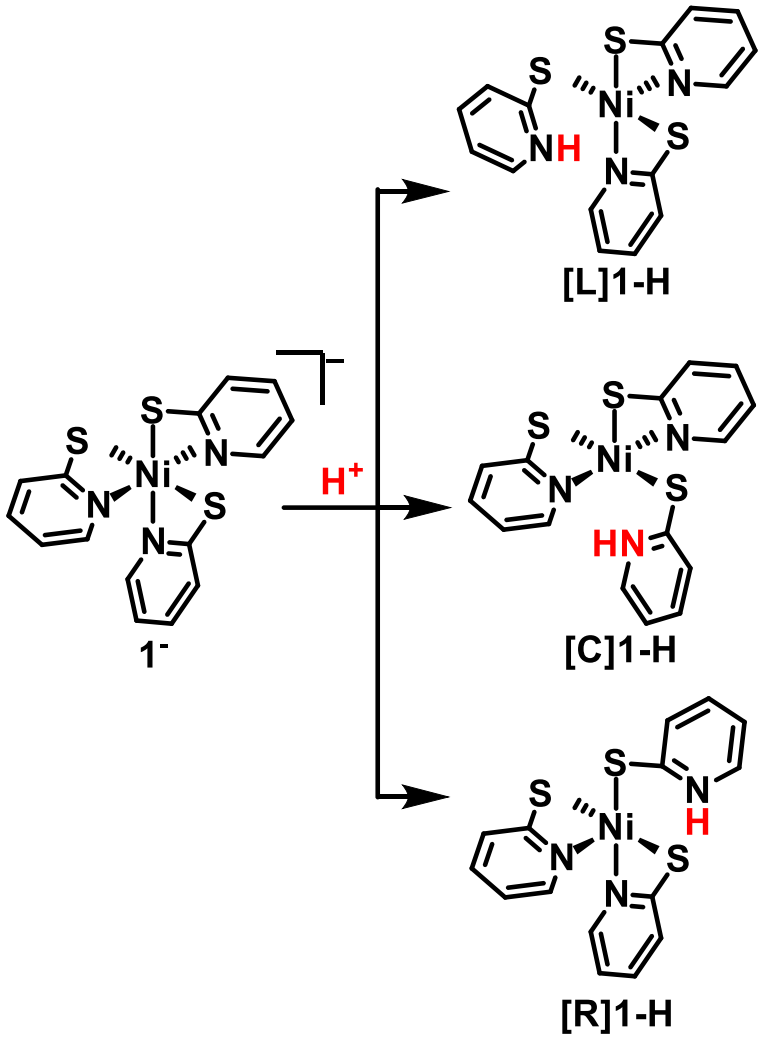
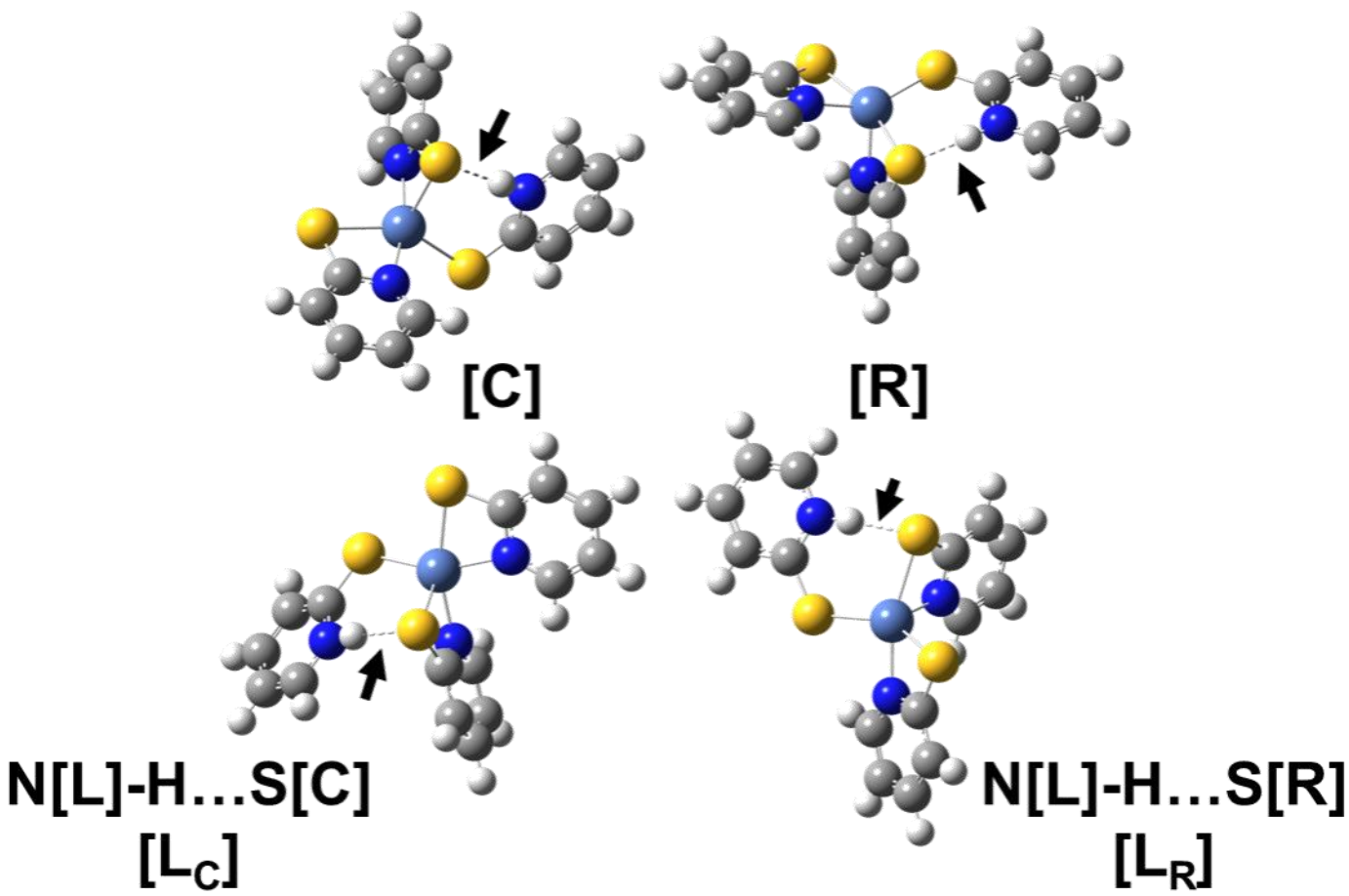
Protonation of Ni(II) catalyst: *Expectation v. Reality*





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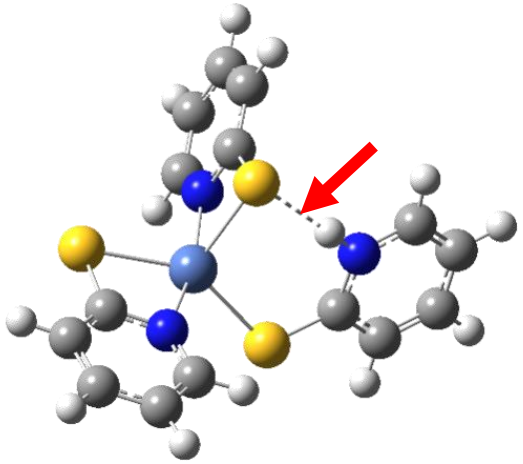
Difference in isomer stability and property

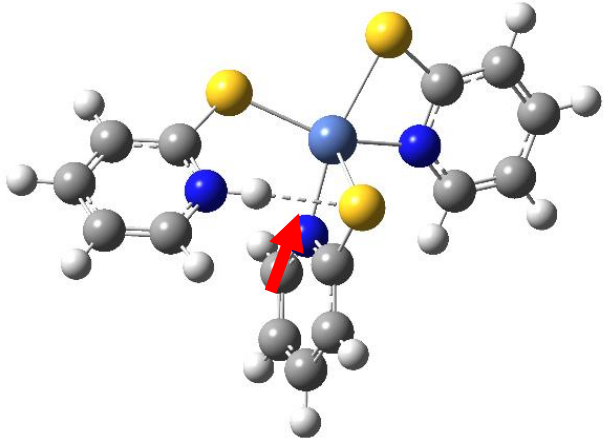


[C]

pK_a = 11.4

%x = 5.27

E^{HB} = -6.32 kcal/mol



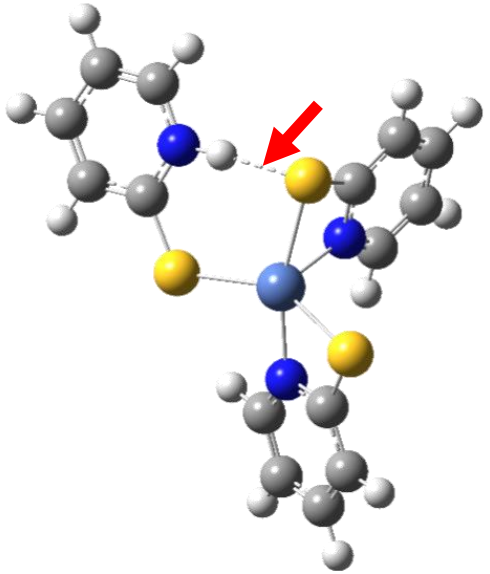
N[L]-H…S[C]

[L_C]

pK_a = 11.1

%x = 2.51

E^{HB} = -5.99 kcal/mol



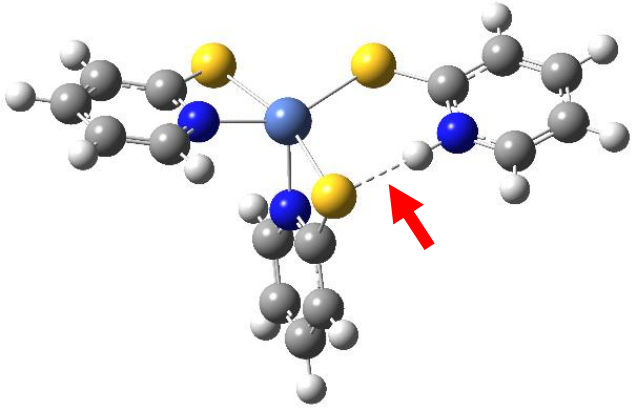
N[L]-H…S[R]

[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

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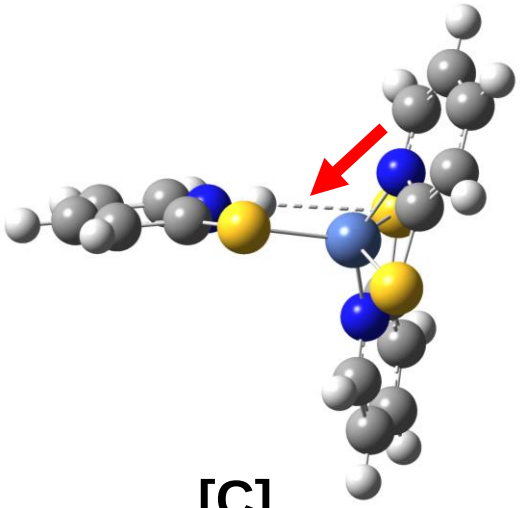
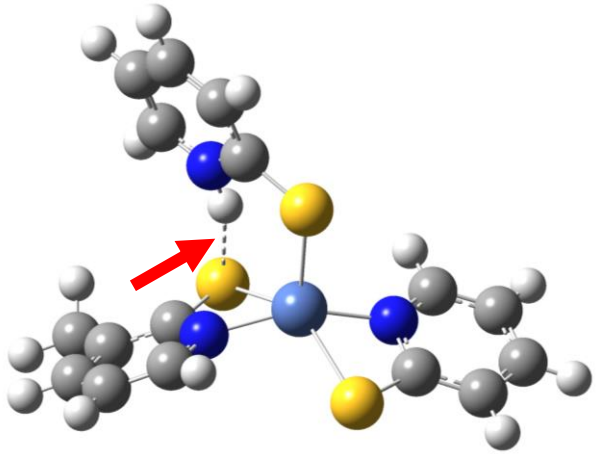
Reduction step of the catalysis



[C]

%x = 44.29

E^{HB} = -6.06 kcal/mol

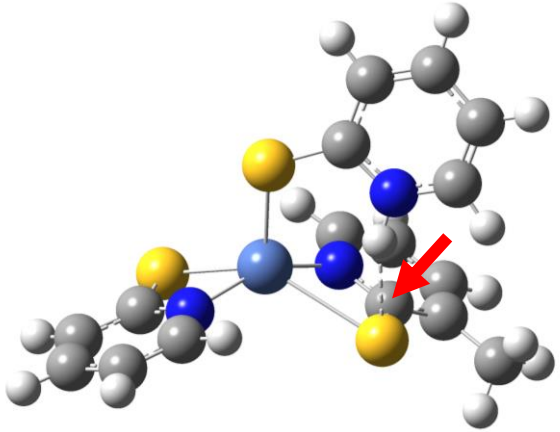


N[L]-H…S[C]

[L_C]

%x = 8.39

E^{HB} = -6.39 kcal/mol

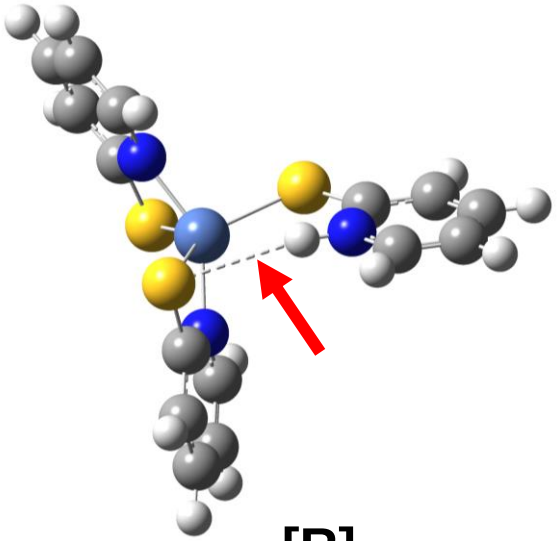


N[L]-H…S[R]

[L_R]

%x = 3.72

E^{HB} = -6.49 kcal/mol



[R]

%x = 43.59

E^{HB} = -6.06 kcal/mol

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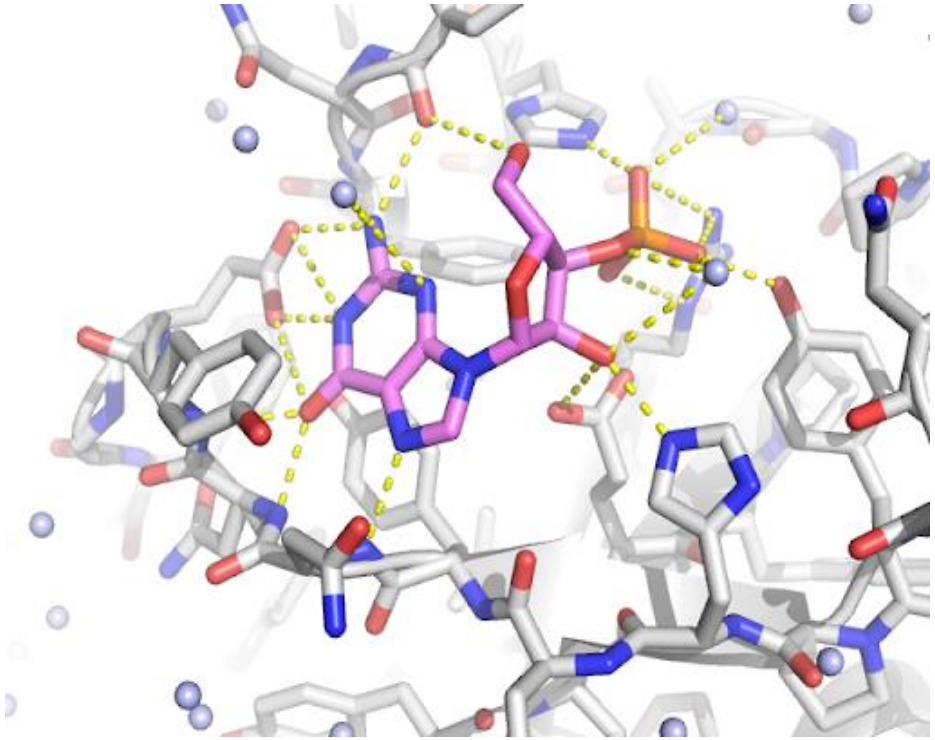
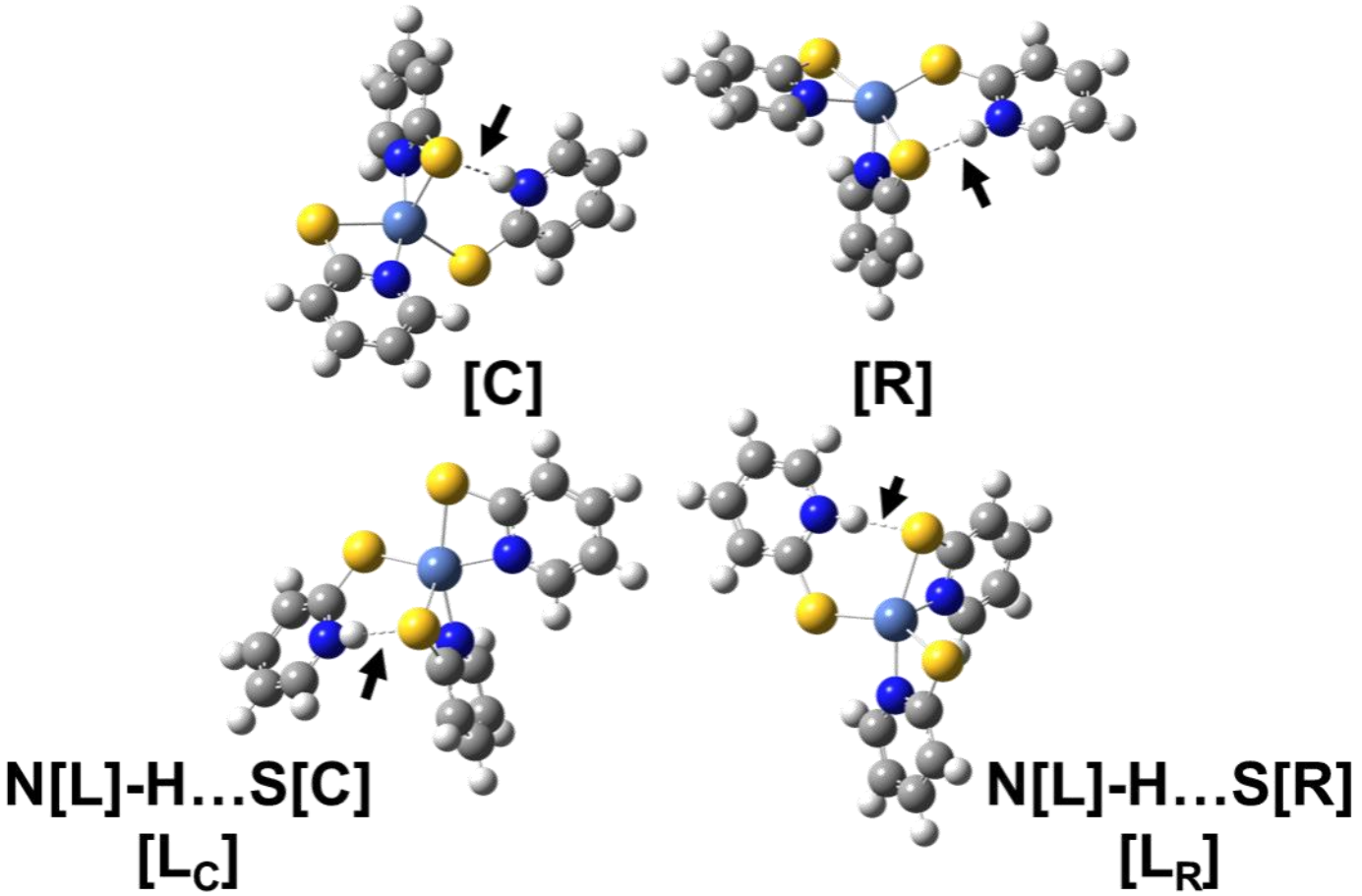
Importance of intramolecular H-bonding in small molecules





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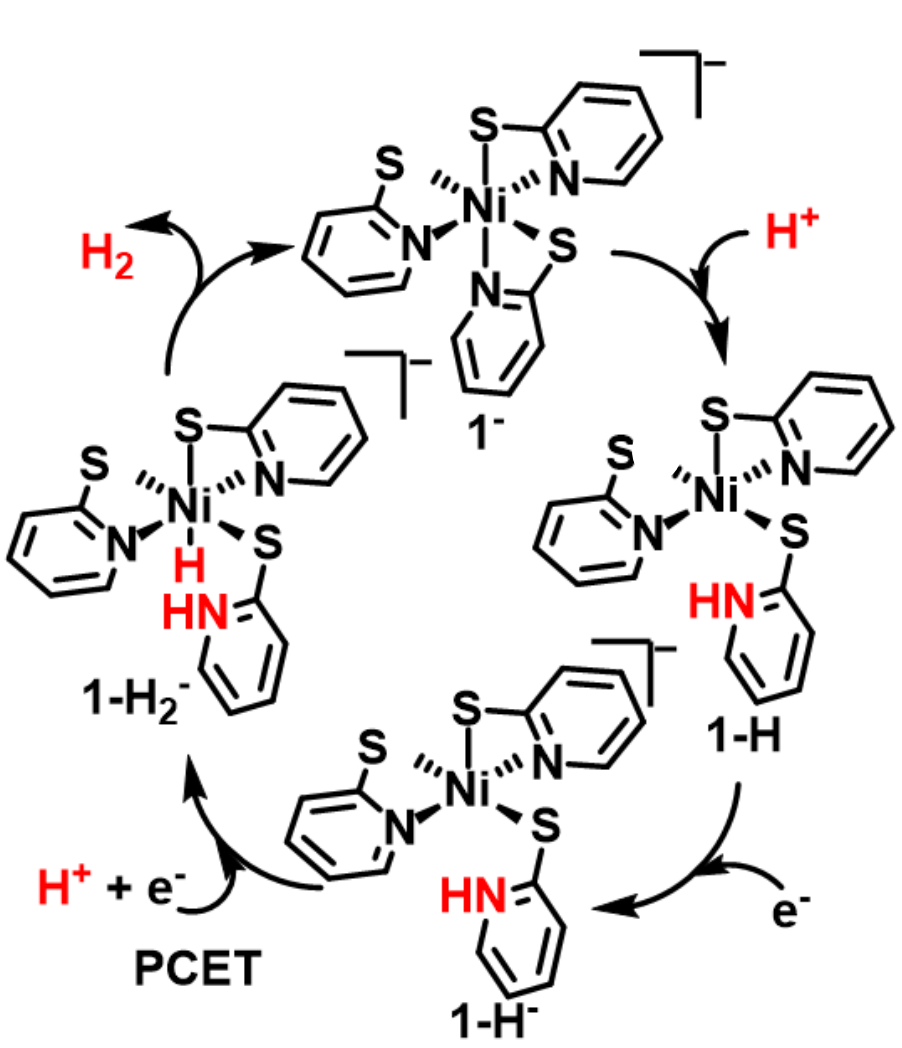
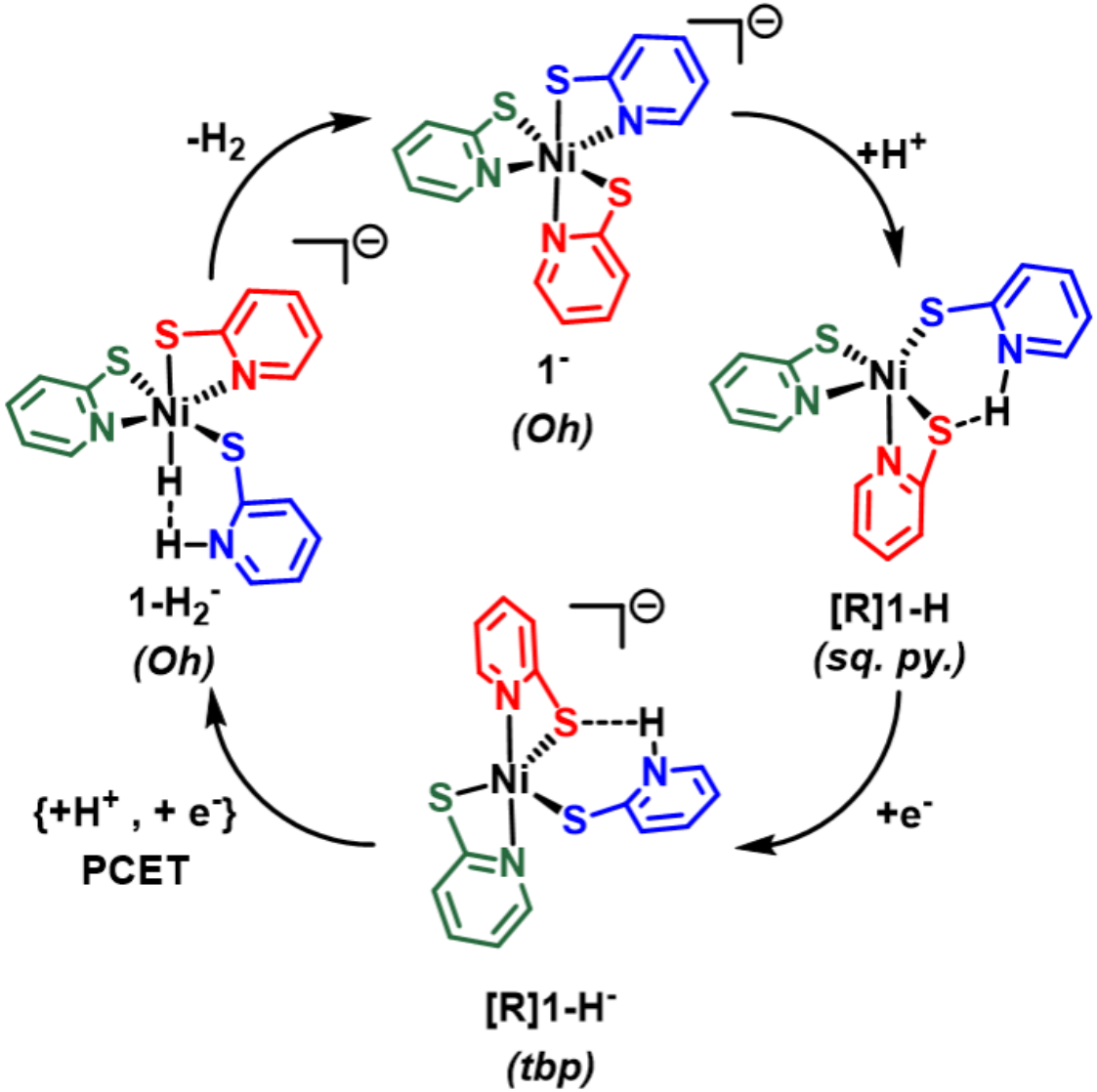
Effect of H-bonding on the catalytic cycle





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Thank you

Dr. Theresa McCormick
Dayalis S. V. Brown
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Prof. Eric Rivard
Dr. Kodi Beyeh
Dr. David Stuart