



# The How to Give a Talk Talk

Christopher J. Cramer

*University of Minnesota, March 6, 2014*



## What's at Stake When You Give a Talk?

Everything!

A job candidate lives or dies in that one hour

In my personal experience, 75% of all talks are a waste of my time

Instead of fearing the risk, embrace the opportunity for reward...

## Before You Start:

- Know your audience (ask if unsure); pitch general or targeted
- Know your time limit (ask if unsure)
- Know your available technology (ask — ok, you get it...)
- What impression are you trying to make?
- What are you wearing? You're *performing*; costume matters
- Practiced? (It helps until it hurts)

# The Title Slide



*Engaging, Professional — not too long or too technical a title, please — same if you were asked for an abstract*



Christopher J. Cramer (and co-workers — thank early)

*University of Minnesota, March 20, 2012*



## My Secrets After 20 Years

- A good talk is a story-telling performance. Imagine telling a story to your favorite 7-year old, and shoot for *that style*.
- Less is more. Your audience will give you far more credit for a shorter story, *that they really felt like they understood*, than they will for a turgid trilogy that just blew by them.
- It is entirely likely that you know more about your science than anyone else in the room. Bring them up to speed in a methodical and informative manner. Teach to Jethro!
- Never run long. *Never*. It's disrespectful, and it illustrates your complete inability to plan. If you have to cut material, then cut it — even on the fly. (I assume 2.5 minutes per slide — get to know your own number with practice.)

# Organization After That Title Slide

- An outline? Why? Are you expecting someone to leave?
- Big picture, introductory material. Why the hell should I, a person outside your research group, give a damn about what you're about to tell me? Why might a funding agency, or humanity in general, care?
- Any really critical discussion of instruments, techniques, spectral interpretation, or other non-generally-well-known concepts that will permeate your talk *if and only if* you can actually get that across in a modest time window
- Narrative results. Interim conclusions (if helpful). More results. More conclusions. Circle back to your big picture. What are the remaining open questions? What's next?

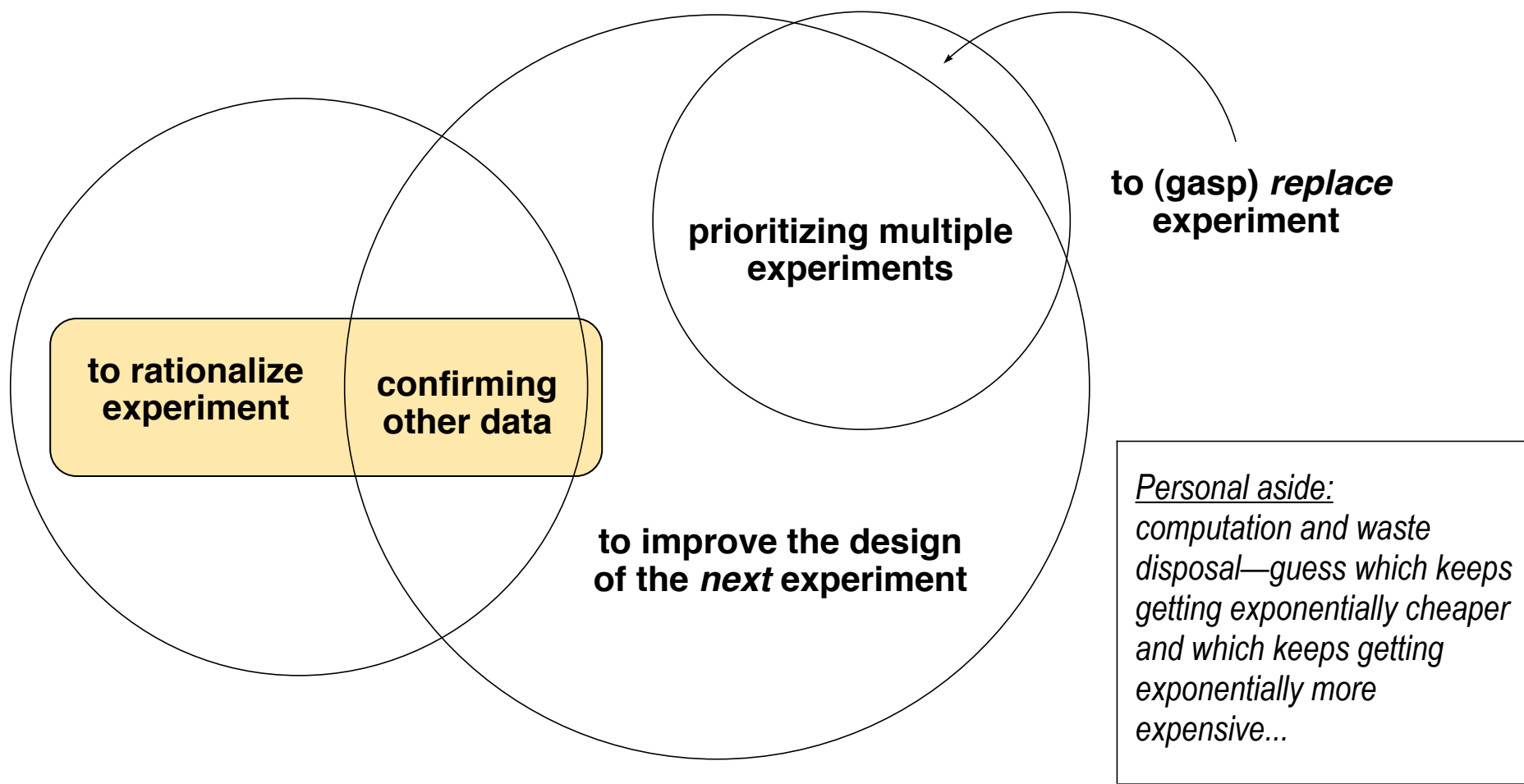
## Organization After That Title Slide

- Big picture, introductory material. Students in particular like this — they may not remember exactly what *you* were doing, but they'll remember that they learned something new from a big picture perspective.

# A One-Slide Summary of Computational Chemistry

*(aka: theoretical chemistry, molecular modeling)*

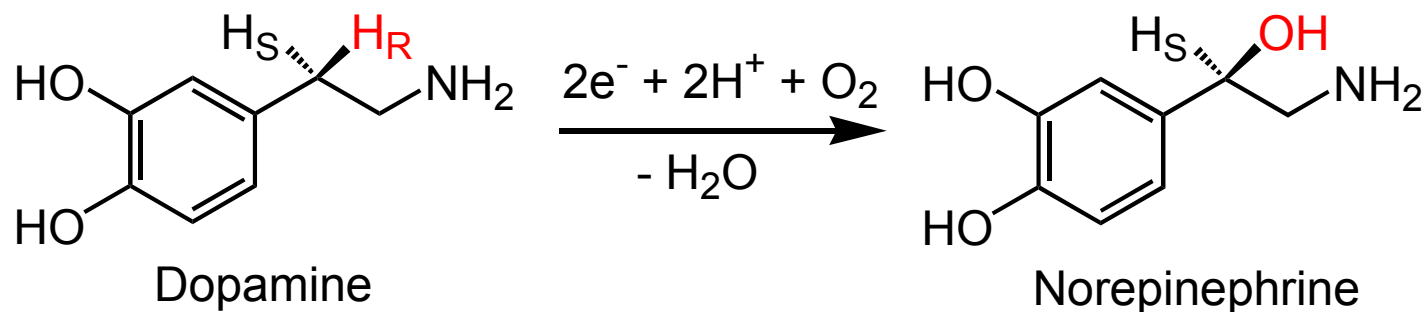
**Why do it?**



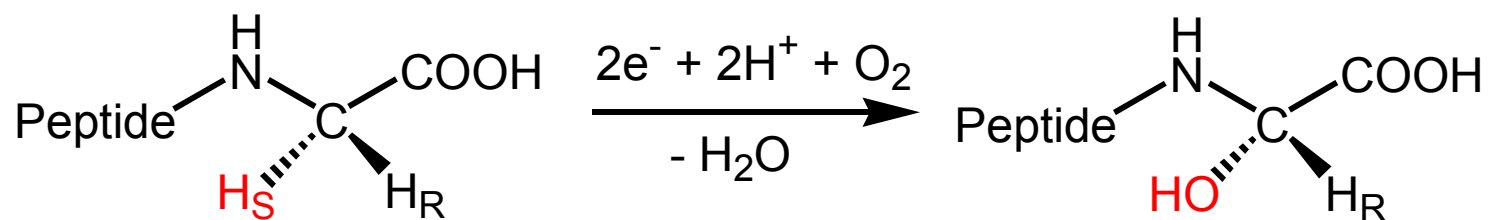


# Dioxygen Activation at Monocopper Sites

## Dopamine $\beta$ -Monooxygenase (D $\beta$ M)

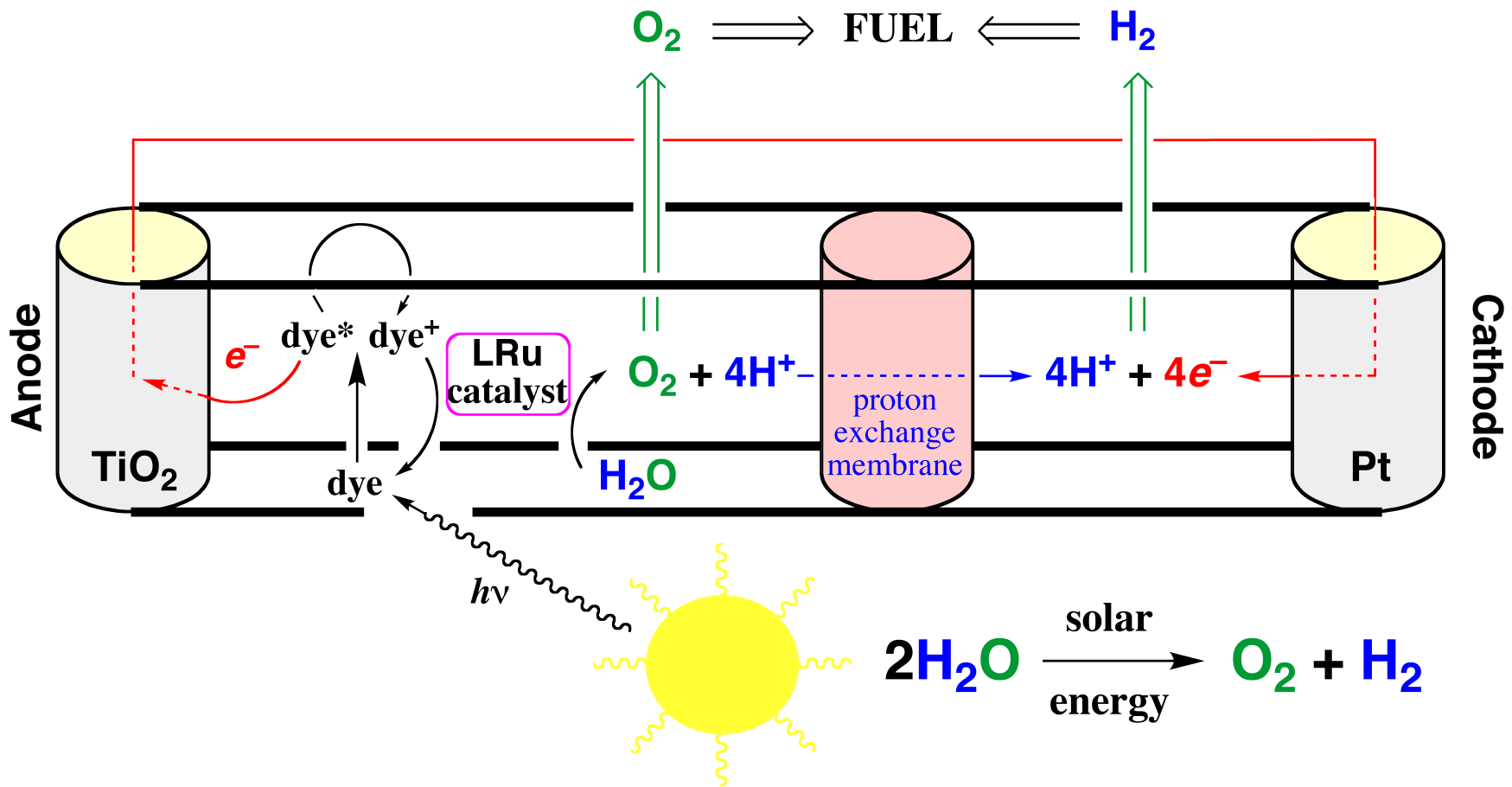


## Peptidylglycine $\alpha$ -Hydroxylating Monooxygenase (PHM)

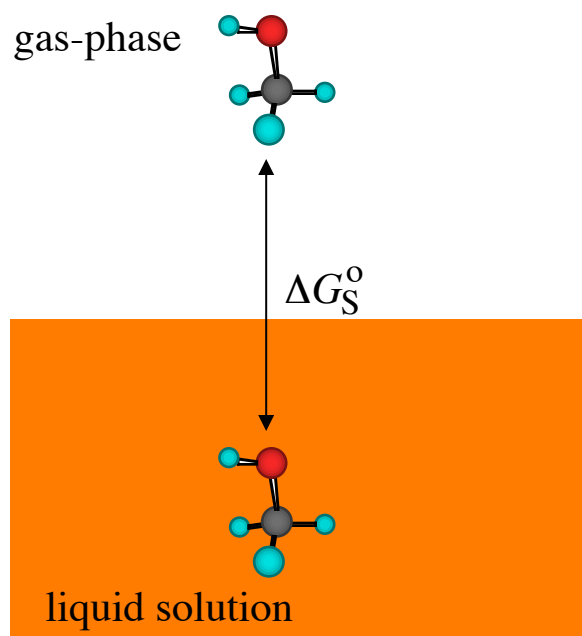


# Conversion of Solar Energy to Green Fuel

## Schematic of the Dye-Sensitized Solar Cell

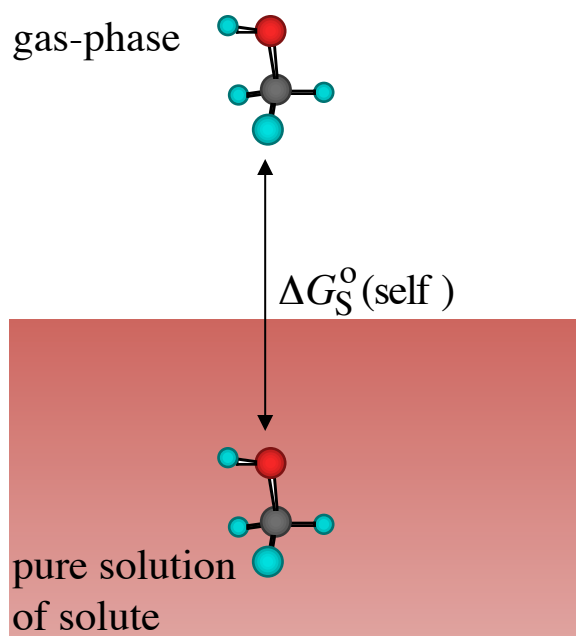


# What Do We Predict with SMx Solvation Models?



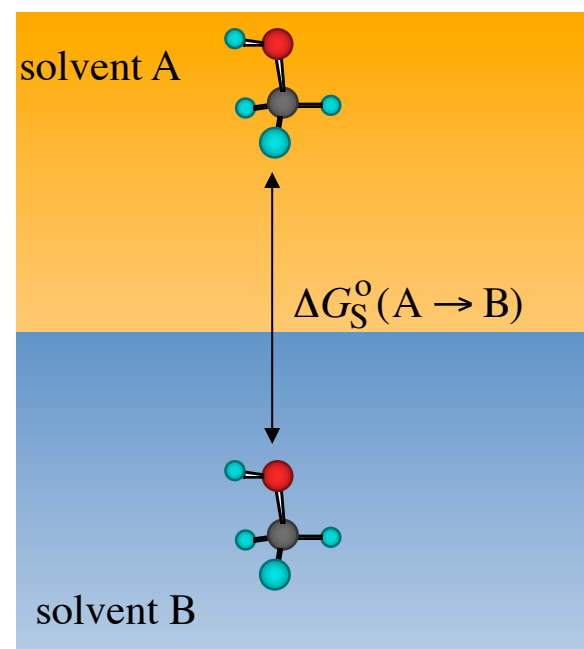
Absolute free energy of solvation

Solvation free energy —  
all solvents, no types



Free energy of self-solvation

Vapor pressure



Transfer free energy of solvation

Partition coefficient

By combining these, we also calculate solubility.

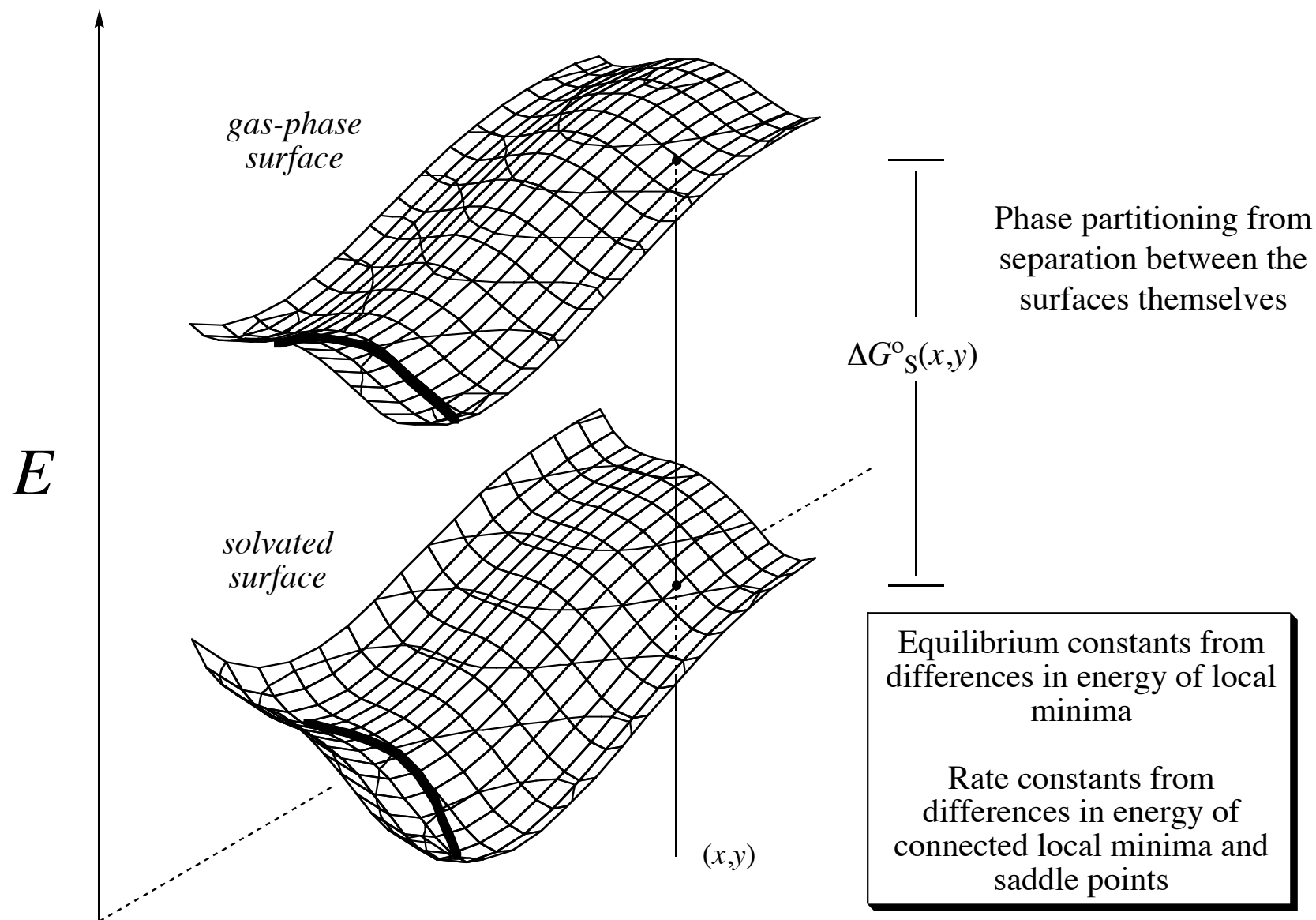
*Have also extended to:*

- *Interface adsorption*
- *Membrane permeability*

# Organization After Those Introductory Slides

- Any really critical discussion of instruments, techniques, spectral interpretation, or other non-generally-well-known concepts that will permeate your talk *if and only if* you can actually get that across in a modest time window

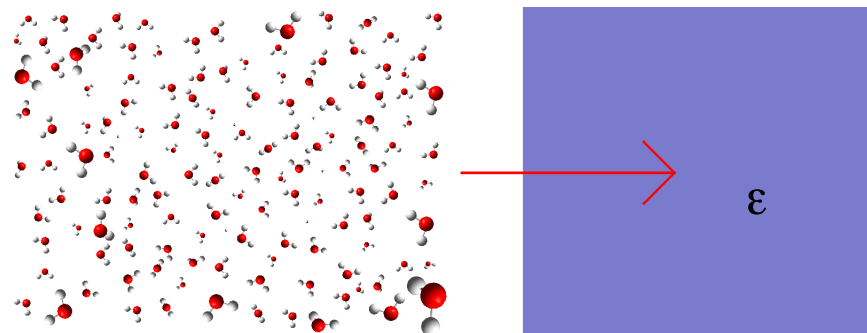
# Potential Energy Surface Perspective



# SMx Bulk Electrostatic Effects

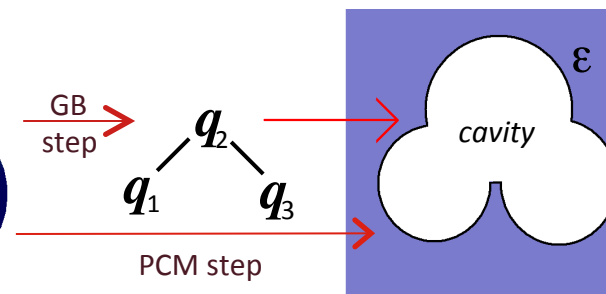
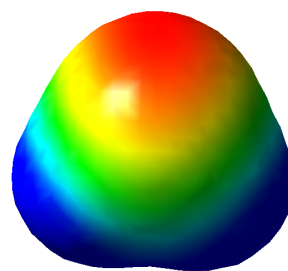
Generalized Born (GB) equation

$$G_P = -\frac{1}{2} \left( 1 - \frac{1}{\epsilon} \right) \sum_{kk'}^{atoms} q_k \gamma_{kk'} q_{k'}$$



Polarized Continuum Model (PCM) equation

$$G_P = -\frac{1}{2} \left( \langle \Psi | V_{RF} | \Psi \rangle + \sum_k^{nuclei} Z_k V_{RF} \right)$$



Limiting behaviors...

Reaction field—usually

$$V_{RF}(\mathbf{r}) = \sum_{k'} \frac{q'_{k'}}{|\mathbf{r} - \mathbf{r}_{k'}|}$$

$r_{kk'} \gg 0$

$$G_P = -\frac{1}{2} \left( 1 - \frac{1}{\epsilon} \right) \frac{q_k q_{k'}}{r_{kk'}}$$

*Coulomb's Law*  
1/2(-gas + solution)

$r_{kk'} = 0$

$$G_P = -\frac{1}{2} \left( 1 - \frac{1}{\epsilon} \right) \frac{q_k^2}{\alpha_k}$$

*Born's Equation*  
monatomic ion

## Pet Peeve

- If you can't explain an equation fully — every term — then leave it out. If you just have to have it, devote the necessary time to explain it. You'll lose half the audience with your first equation that flashes by with an inadequate explanation. Your job is to make the equation seem *intuitive*.

The same holds true for reagent acronyms in synthetic schemes... Spectra with unexplained features... etc.

In sum, if you put it on the slide, explain it. If you aren't going to explain it, why did you put it on the slide? To show off how smart you are? Bad move...

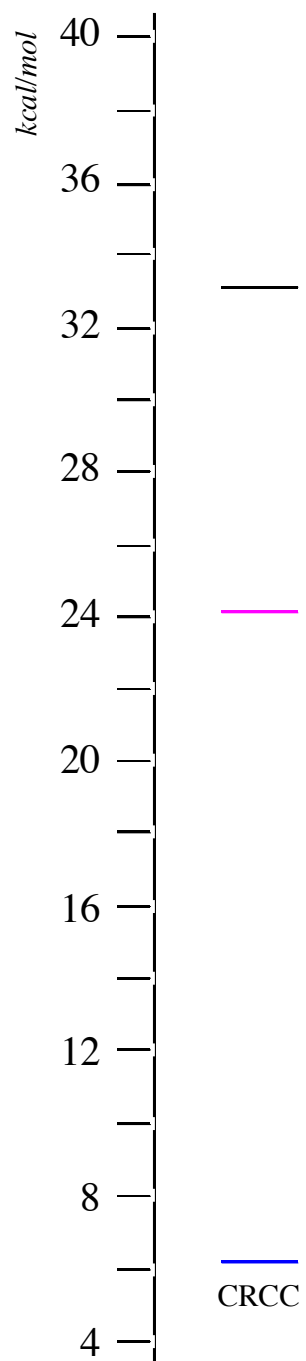
# Impressive? Yes. Interesting? No.

$$\begin{aligned}
 \frac{\partial q_k}{\partial P_{\mu\nu}} &= \delta_{\mu\nu} \left[ \delta_{kk(\mu)} (-1 - B_k c_k) + (1 - \delta_{kk(\mu)}) B_{kk(\mu)} c_{k(\mu)} \right] \\
 &+ \left( 1 - \delta_{k(\mu)k(\nu)} \right) \left\{ \begin{aligned} &\left( 1 - \delta_{kk(\mu)} \right) \left( 1 - \delta_{kk(\nu)} \right) \left[ \begin{aligned} &- B_{kk(\mu)} \left( \delta_{k(\mu)H} P_{\mu\nu} d_{Hk(\nu)} + \delta_{k(\mu)O} P_{\mu\nu} d_{Ok(\nu)} \right) \\ &- B_{kk(\nu)} \left( \delta_{k(\nu)H} P_{\mu\nu} d_{Hk(\mu)} + \delta_{k(\nu)O} P_{\mu\nu} d_{Ok(\mu)} \right) \end{aligned} \right] \\ &+ \delta_{kk(\mu)} \left\{ \begin{aligned} &P_{\mu\nu} \left[ c_k q_k^{(0)} + (1 - \delta_{kH}) d_k + \delta_{kH} \sum_{k' \neq k} B_{kk'} d_{Hk'} + \delta_{kO} \sum_{k' \neq k} B_{kk'} d_{Ok'} \right] \\ &+ \delta_{kk(\mu)} \left\{ \begin{aligned} &B_k \left( \delta_{kH} P_{\mu\nu} d_{Hk(\nu)} + \delta_{kO} P_{\mu\nu} d_{Ok(\nu)} \right) \\ &- P_{\mu\nu} \left[ \begin{aligned} &c_{k(\nu)} q_{k(\nu)}^{(0)} + (1 - \delta_{k(\nu)H}) d_{k(\nu)} \\ &+ \delta_{k(\nu)H} \sum_{k' \neq k(\nu)} B_{k(\nu)k'} d_{Hk'} + \delta_{k(\nu)O} \sum_{k' \neq k(\nu)} B_{k(\nu)k'} d_{Ok'} \end{aligned} \right] \end{aligned} \right\} \\ &+ \left( \delta_{kk(\mu)} + \delta_{kk(\nu)} \right) \left\{ \begin{aligned} &- B_{kk(\nu)} \left( \delta_{k(\nu)H} P_{\mu\nu} d_{Hk} + \delta_{k(\nu)O} P_{\mu\nu} d_{Ok} \right) \\ &+ \delta_{kk(\nu)} \left\{ \begin{aligned} &B_k \left( \delta_{kH} P_{\mu\nu} d_{Hk(\mu)} + \delta_{kO} P_{\mu\nu} d_{Ok(\mu)} \right) \\ &- P_{\mu\nu} \left[ \begin{aligned} &c_{k(\mu)} q_{k(\mu)}^{(0)} + (1 - \delta_{k(\mu)H}) d_{k(\mu)} \\ &+ \delta_{k(\mu)H} \sum_{k' \neq k(\mu)} B_{k(\mu)k'} d_{Hk'} + \delta_{k(\mu)O} \sum_{k' \neq k(\mu)} B_{k(\mu)k'} d_{Ok'} \end{aligned} \right] \end{aligned} \right\} \\ &- B_{kk(\mu)} \left( \delta_{k(\mu)H} P_{\mu\nu} d_{Hk} + \delta_{k(\mu)O} P_{\mu\nu} d_{Ok} \right) \end{aligned} \right\} \end{aligned} \right\}
 \end{aligned}$$



## Some Technical Things

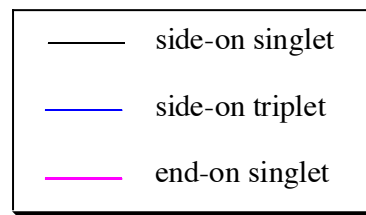
- You've already seen how I like bulleted text.
- Slide backgrounds: Keep 'em simple. Unless you're selling worthless stocks, you want your audience focused on your slides' *contents*, not some fabulous wallpaper that you also proudly use on your Twitter homepage.
- If you do want to appear and disappear things (which can definitely be a useful way to focus your audience's attention!), keep it simple: on/off, or maybe grayout in certain instances. Avoid garish spinning, sliding, exploding, etc.
- Font sizes. Never, ever less than 14 pt on a landscape slide, and that small only for citations, for example. If it won't all fit on one slide, you've got too much on the slide...



$\text{CuO}_2^+$   
 $\Delta E_{\text{rel}}$  to end-on triplet

*bold line = restricted DFT*

*thin line = broken-symmetry spin-purified DFT*



# Tabular data

- Is there a number you don't plan to mention? Then why did you display it?
- Bigger fonts are better.
- Highlight the most important data where warranted.
- Keep borders clean and simple

# SM8 Performance (OK table)

Mean unsigned errors (kcal/mol) for SM8 and some other popular continuum solvation models

Solute class	Data	SM8	<u>IEF-PCM</u>	C-PCM	PB	All equal
	<i>N</i>		<i>G03/UA0</i>	<i>GAMESS</i>	<i>Jaguar</i>	to mean
aqueous neutrals	274	<b>0.5</b>	<b>4.9</b>	1.6	0.9	2.7
nonaq. neutrals	666	<b>0.6</b>	<b>6.0</b>	<b>2.8</b>	<b>2.3</b>	1.5
aqueous ions	112	<b>3.2</b>	<b>12.4</b>	8.4	4.0	8.6
nonaqueous ions	220	<b>4.9</b>	8.4	8.4	8.1	8.6

Cramer, C. J.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 760

Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. "Performance of SM6, SM8, and SMD on the SAMPL1 Test Set for the Prediction of Small-Molecule Solvation Free Energies" *J. Phys. Chem. B* **2009**, *113*, 4538.

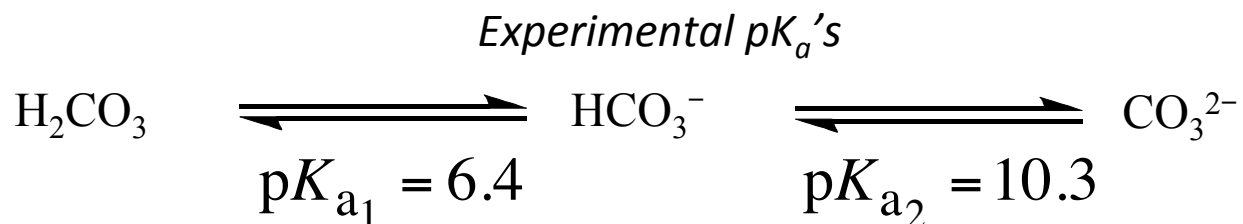
Ribeiro, R. F.; Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. "Prediction of SAMPL2 Aqueous Solvation Free Energies and Tautomeric Ratios Using the SM8, SM8AD, and SMD Solvation Models" *J. Comput.-Aid. Mol. Des.* **2010**, *24*, 317.

# SM8 Performance (Poor table)

compound	SM8	exp
uracil	-16.76	-16.59 ± 0.28
5-bromouracil	-16.39	-18.17 ± 0.55
5-chlorouracil	-16.59	-17.74 ± 0.78
5-fluorouracil	-17.38	-16.92 ± 0.88
5-trifluoromethyluracil	-16.52	-15.46 ± 0.16
6-chlorouracil	-14.24	-15.83 ± 1.22
cyanuric acid	-20.32	-18.26 ± 0.27
caffeine	-11.90	-12.64 ± 0.74
methyl paraben	-9.85	-9.51 ± 0.26
ethyl paraben	-9.50	-9.20 ± 0.30
propyl paraben	-9.24	-9.37 ± 0.22
butyl paraben	-8.42	-8.72 ± 0.27
acetylsalicylic acid	-11.93	-9.94 ± 0.18
diflunisal	-13.96	-9.40 ± 0.20
flurbiprofen	-9.03	-8.42 ± 0.16
ibuprofen	-6.88	-7.00 ± 0.64
ketoprofen	-12.56	-10.78 ± 0.18
naproxen	-10.90	-10.21 ± 0.18
phthalimide	-11.99	-9.61 ± 0.50
sulfolane	-13.26	-8.61 ± 0.31
<b>D-glucose</b>	<b>-25.29</b>	<b>-25.47 ± 0.22</b>
<b>D-xylose</b>	<b>-21.71</b>	<b>-20.52 ± 0.27</b>

Ribeiro, R. F.; Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. "Prediction of SAMPL2 Aqueous Solvation Free Energies and Tautomeric Ratios Using the SM8, SM8AD, and SMD Solvation Models" *J. Comput.-Aid. Mol. Des.* **2010**, *24*, 317.

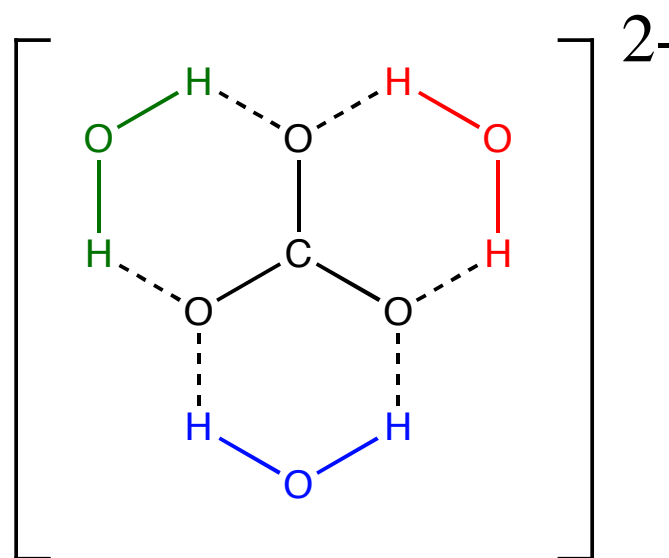
# Adding More Waters (Best Table)



*(nicely multimedia-y)*

*Calculated pK<sub>a</sub>'s*

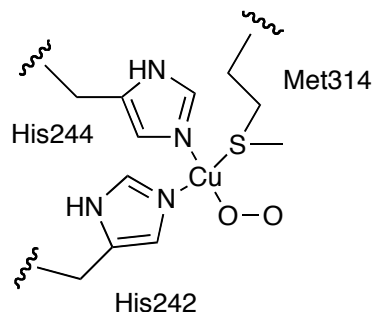
No. H <sub>2</sub> O	pK <sub>a1</sub>	pK <sub>a2</sub>
0	-0.6	1.6
<b>1</b>	<b>1.3</b>	<b>5.0</b>
<b>2</b>	<b>2.3</b>	<b>7.8</b>
<b>3</b>	<b>4.2</b>	<b>9.0</b>



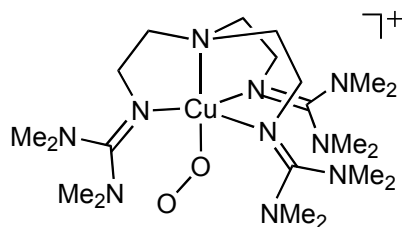
Adding explicit water molecules improves the accuracy of the calculation

# Known LCuO<sub>2</sub> Models—Substantial Diversity

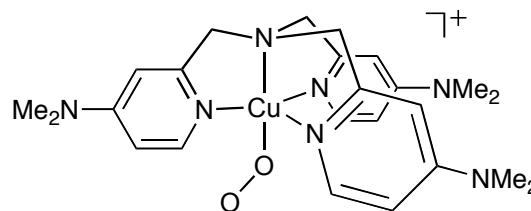
*Ensure all structures are big enough to be easily seen in the back row;  
be consistent in how you draw all structures (bond lengths, fonts)*



PHM precatalytic complex  
 $r_{OO} = 1.23 \text{ \AA}$   
ground state ?

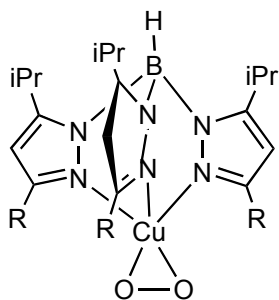


Schindler et al.  
 $r_{OO} = 1.28 \text{ \AA}$   
ground state triplet



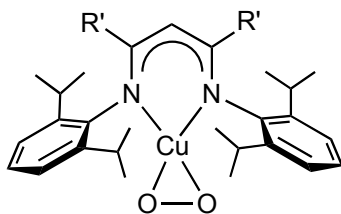
Karlin et al.  
 $r_{OO} = ?$   
ground state ?

*If you need to  
show 3D  
structures,  
consider having  
them rotate  
(looped) to  
improve  
perspective*



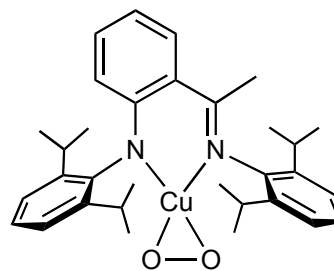
**a**, R = tBu  
**b**, R = Ad

Kitajima et al.  
 $r_{OO} = [1.33] \text{ \AA}$   
ground state singlet



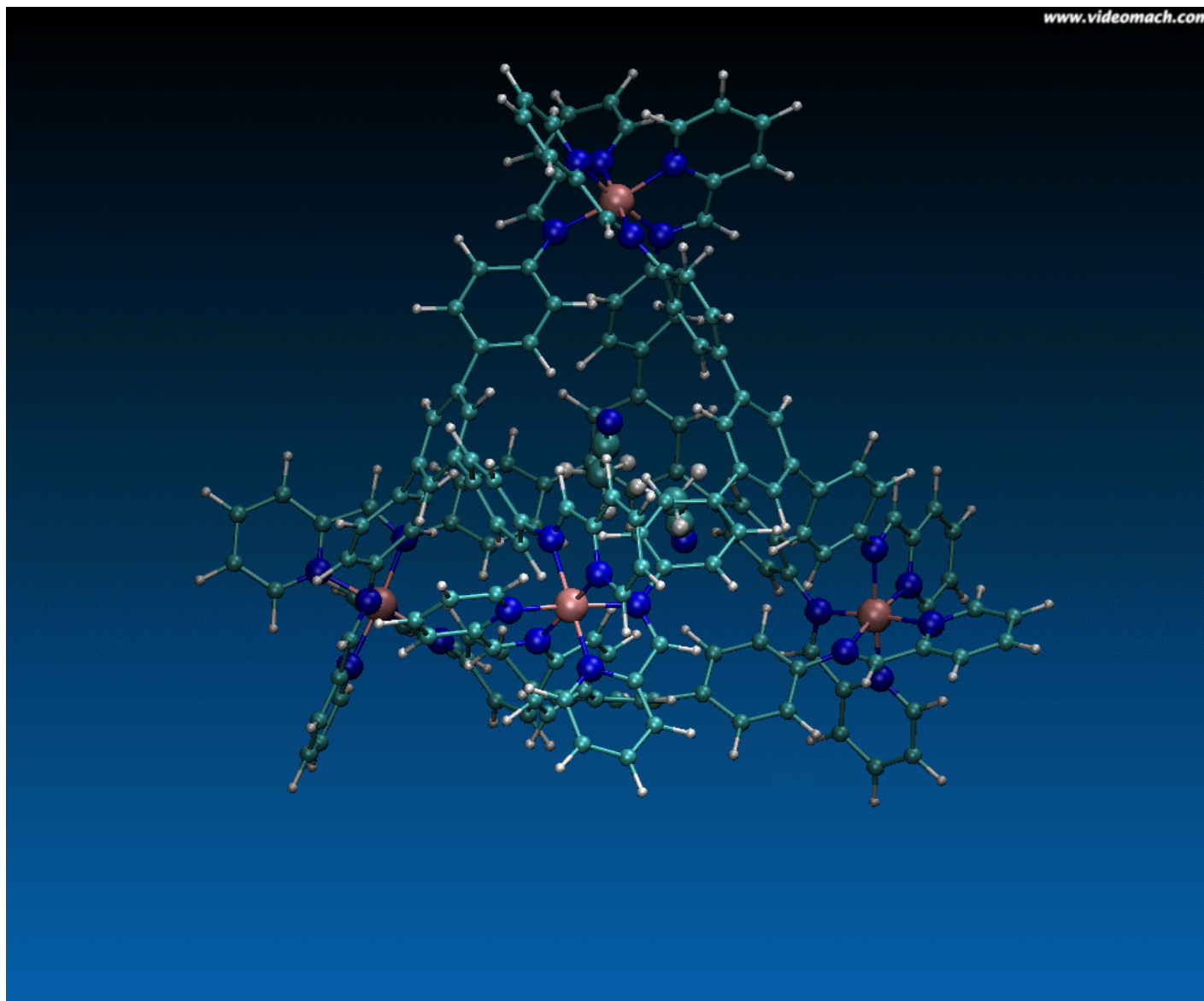
**a**, R' = Me  
**b**, R' = tBu

Tolman et al.  
 $r_{OO} = 1.39 \text{ \AA}$   
ground state singlet



Tolman et al.  
 $r_{OO} = 1.39 \text{ \AA}$   
ground state singlet

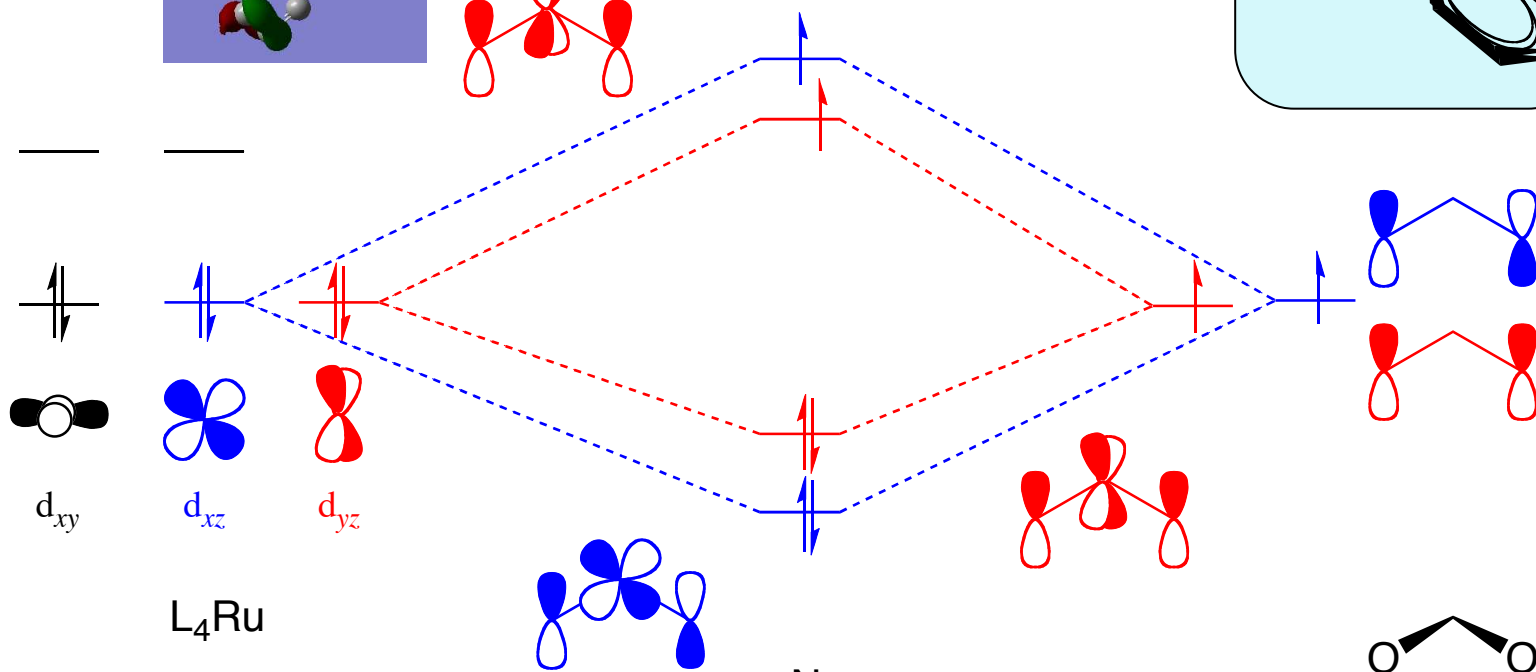
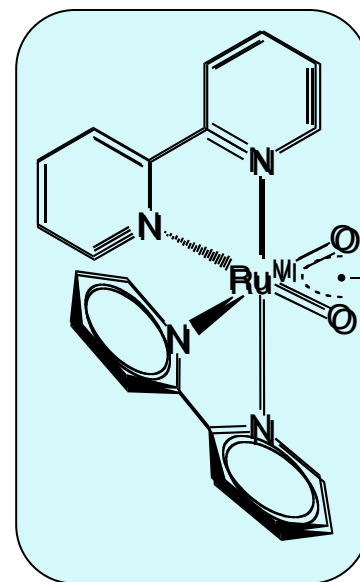
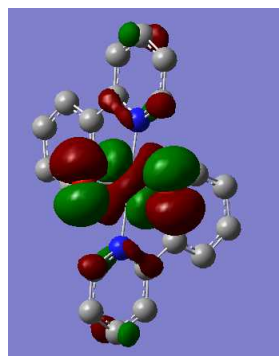
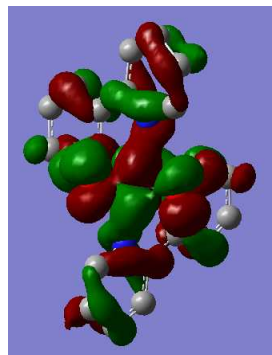
# A Host-Guest System That Needs Animation



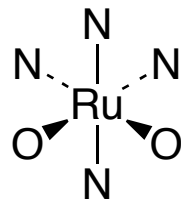


# Oxidation State of Ru?

Triplet  
SOMOs



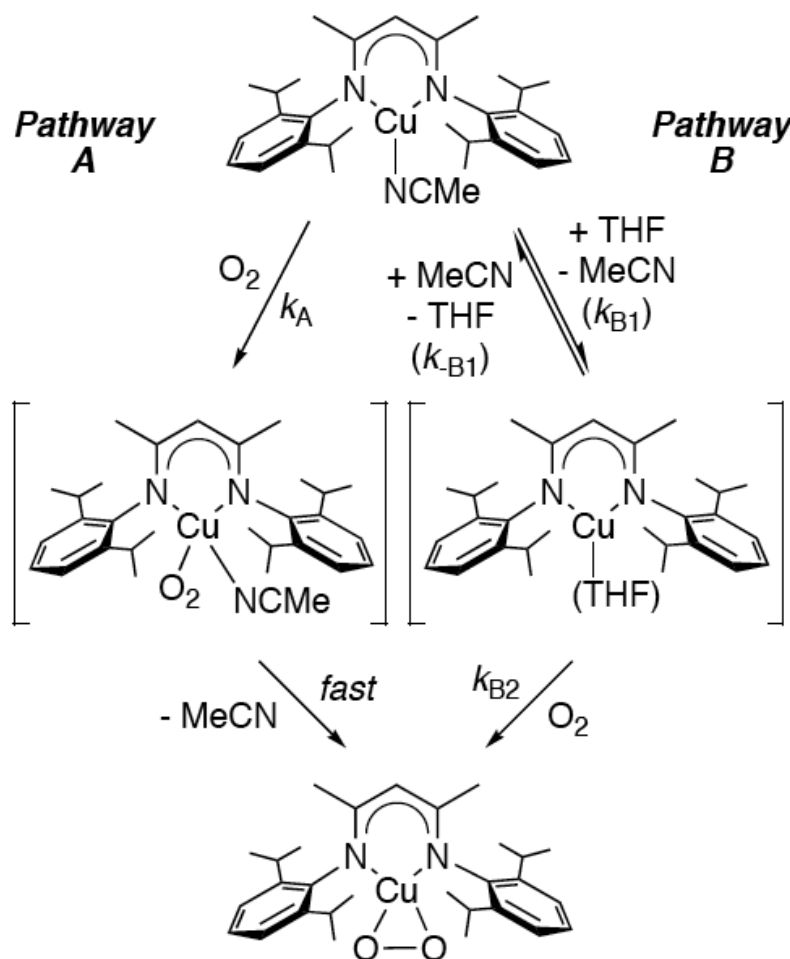
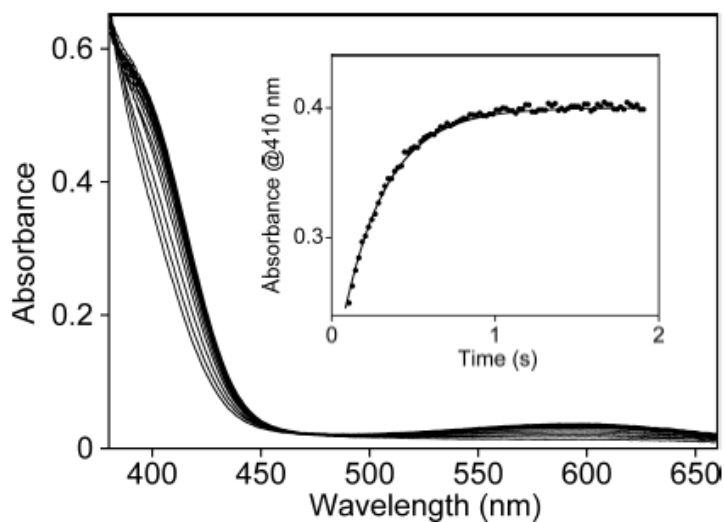
colors are good (within limits)  
highlight boxes are very good to  
organize slides



$\pi$  hybridization of octahedral  $Ru^{II}$   
d orbitals with 2 neutral O atoms

# Stop-flow Kinetics for Oxygenation

Do your best to get all related data, concepts, conclusions, on single slides



$$\frac{\partial [L^1CuO_2]}{\partial t} = k_A [L^1Cu(MeCN)] [O_2] + k_B [L^1Cu(MeCN)]$$

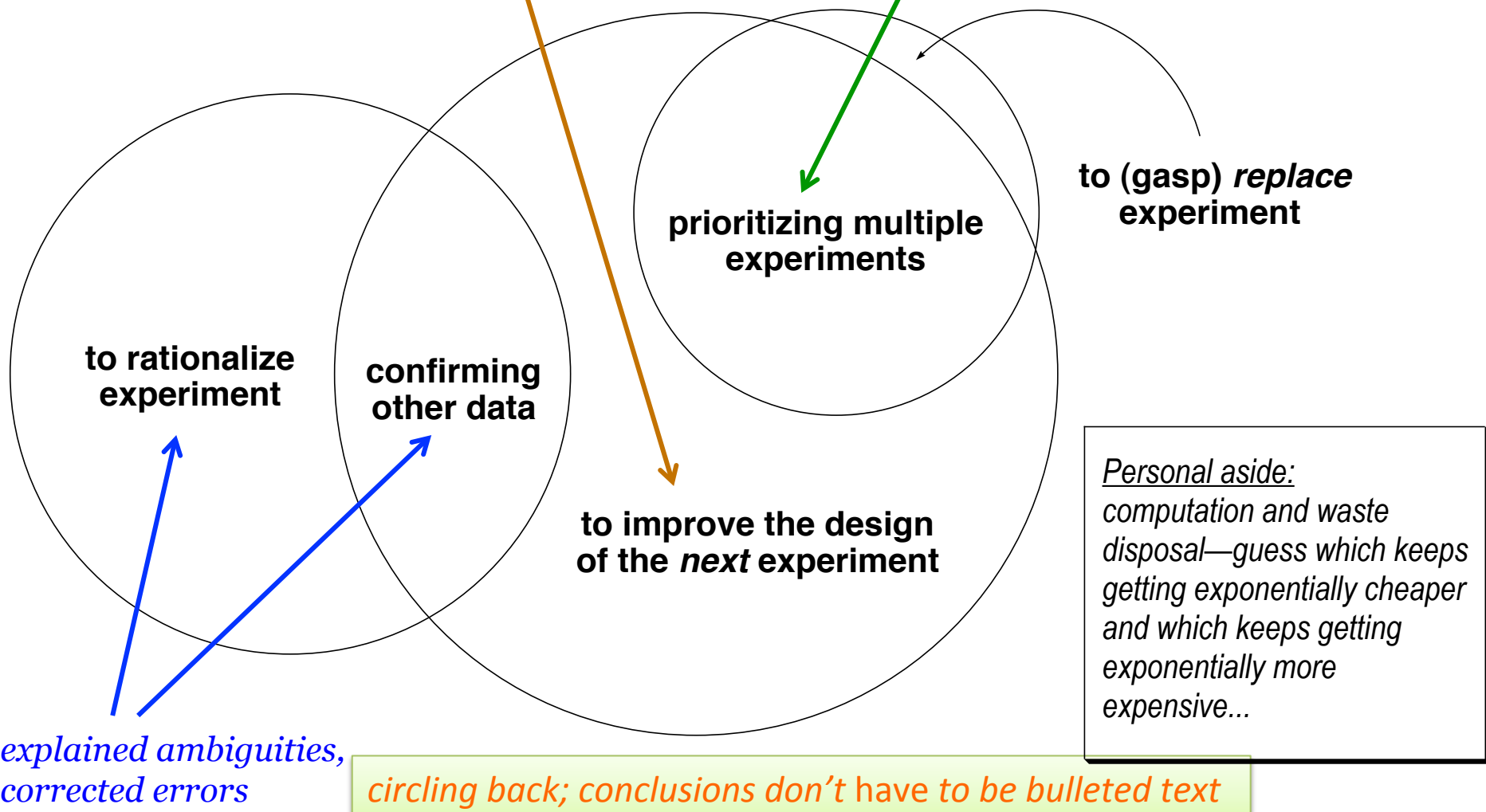
# A One-Slide Summary of Computational Chemistry

*(aka: theoretical chemistry, molecular modeling)*

**Why do it?**

*provided spectral handle on  
O<sub>2</sub> oxidation level*

*validated model can now be used  
to design improved catalysts in  
silico prior to synthetic efforts*



# Acknowledgments

## Oxygen Activation

Dr. Ben Gherman  
Dr. Abdul R. Moughal Shahi  
Dr. Stefan Huber  
Dr. Patrick Donoghue  
Dr. Joe Scanlon  
David Heppner

## Water Splitting/CO<sub>2</sub> Activ.

Dr. Pere Miró  
Dr. Tanya Todorova  
Zahid Ertem  
Nora Planas  
Stuart Kohl

## Senior Collaborators

Prof. Laura Gagliardi  
(Geneva/Minnesota)  
Prof. Shinobu Itoh (Osaka)  
Prof. Antoni Llobet (ICIQ)  
Prof. Piotr Piecuch (MSU)  
Prof. Bill Tolman (Minnesota)



## Dirty Little Secret

- Every rule I've just laid down, I've felt free to violate at one time or another. *But*, only when I've believed the payoff to outweigh the unprofessionalism.

THANKS!!

- Questions welcome