CH40208

TOPICS IN COMPUTATIONAL CHEMISTRY

WHAT IS COMPUTATIONAL CHEMISTRY AND WHY LEARN ABOUT IT?

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- examples:
  - what is the groundstate structure of a molecule?
  - what are a molecule's HOMO & LUMO and how does this affect reactivity?
  - what voltage should we get from a new solar cell material?
  - is this proposed synthesis pathway viable?
  - what does this complex dataset tell us about our chemistry?

EXAMPLES OF COMPUTATIONAL RESEARCH AT BATH

- How does changing chemistry affect the performance of battery materials? (BJM / MSI)
- Predicting the performance of new thermoelectric materials (SJC)
- How do K^+ ions pass through channels in cell membranes? (CD)
- How does zeolite structure affect catalytic properties (AOM)
- What are the energy barriers for competing synthetic pathways? (CLM / MNG)
- What are the magnetic properties of new transition-metal complexes (ES)

NOT JUST THE "COMPUTATIONAL" SECTION

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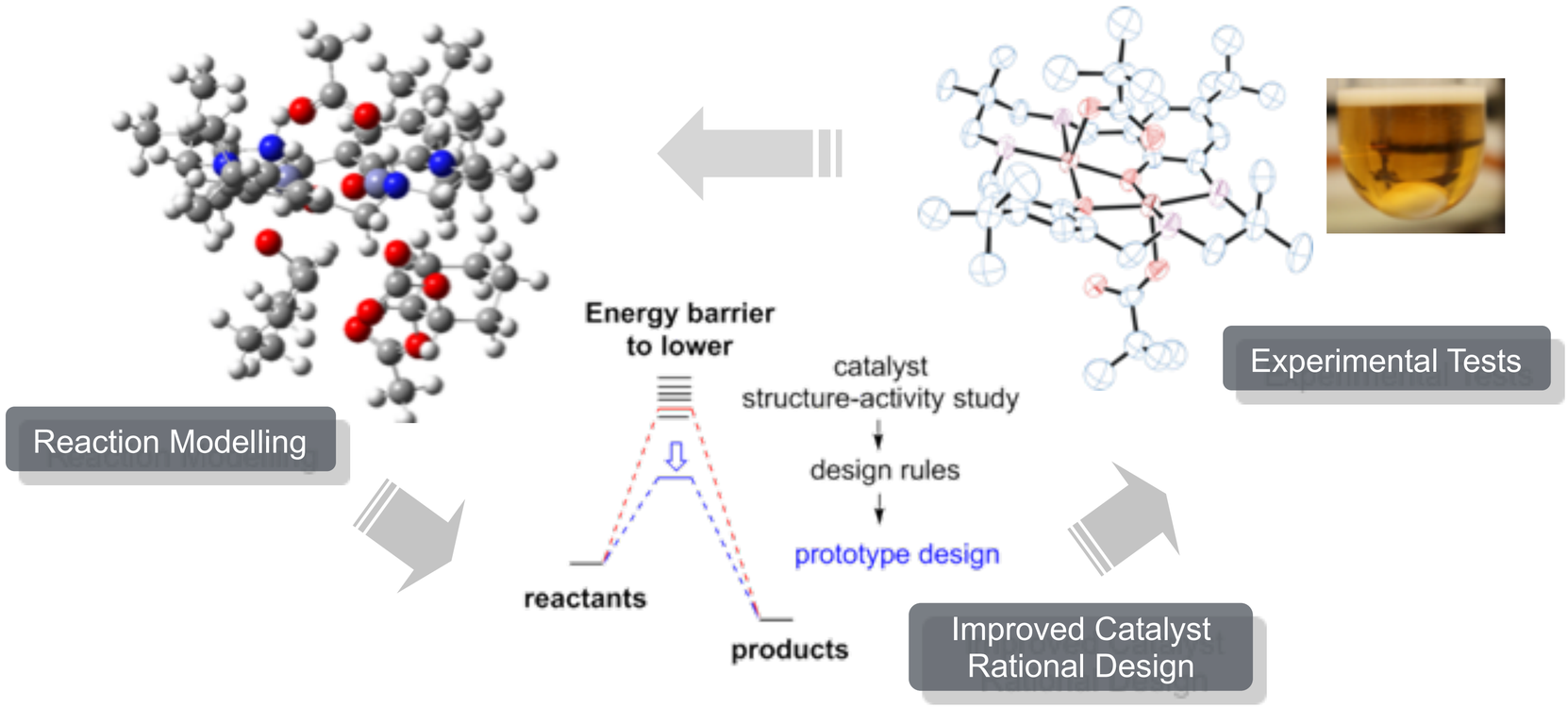
- Antoine Buchard

Understanding/predicting catalyst structure/activity relationship



NOT JUST THE "COMPUTATIONAL" SECTION

- Mike Hill / Mary Mahon (Claire McMullin)

ORGANOMETALLICS

Organocalcium-mediated nucleophilic alkylation of benzene

Andrew S. S. Wilson,[1] Michael S. Hill,[1]* Mary F. Mahon,[1] Chiara Dinoi,[2] Laurent Maron[2]*

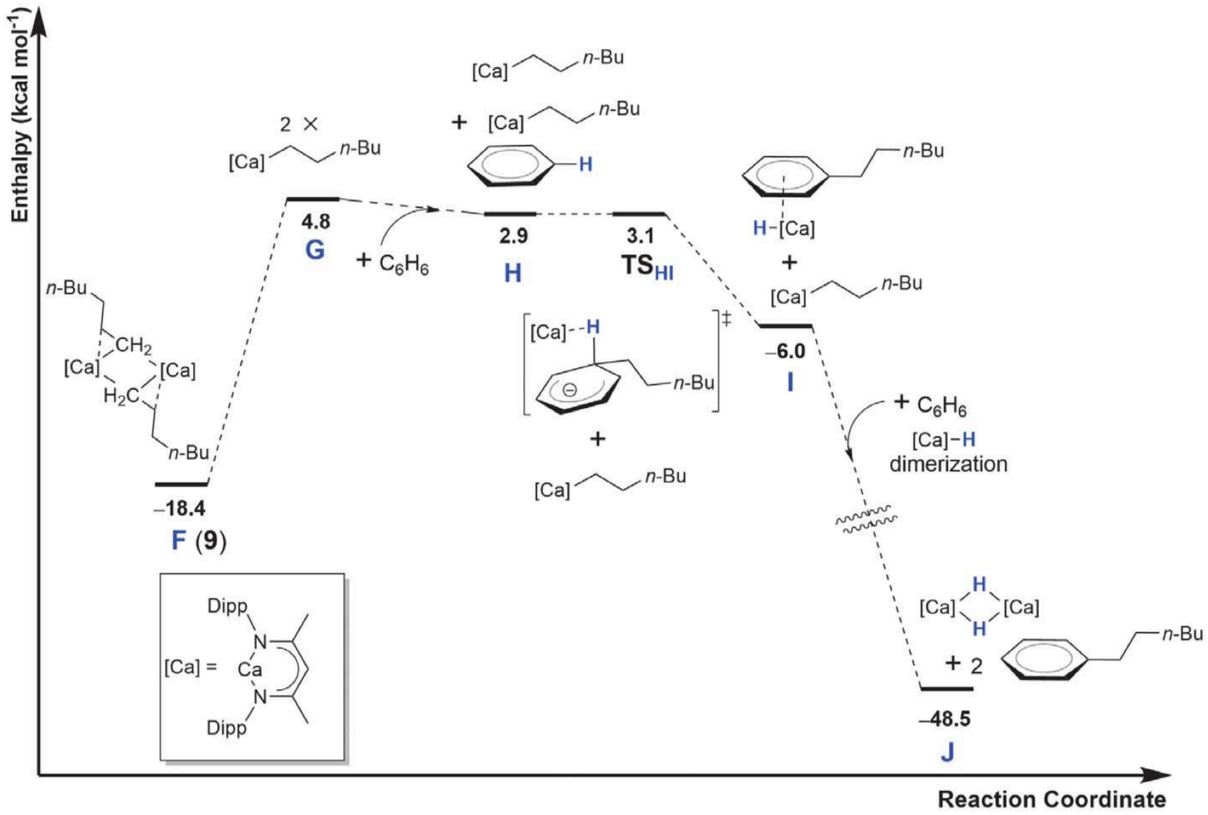
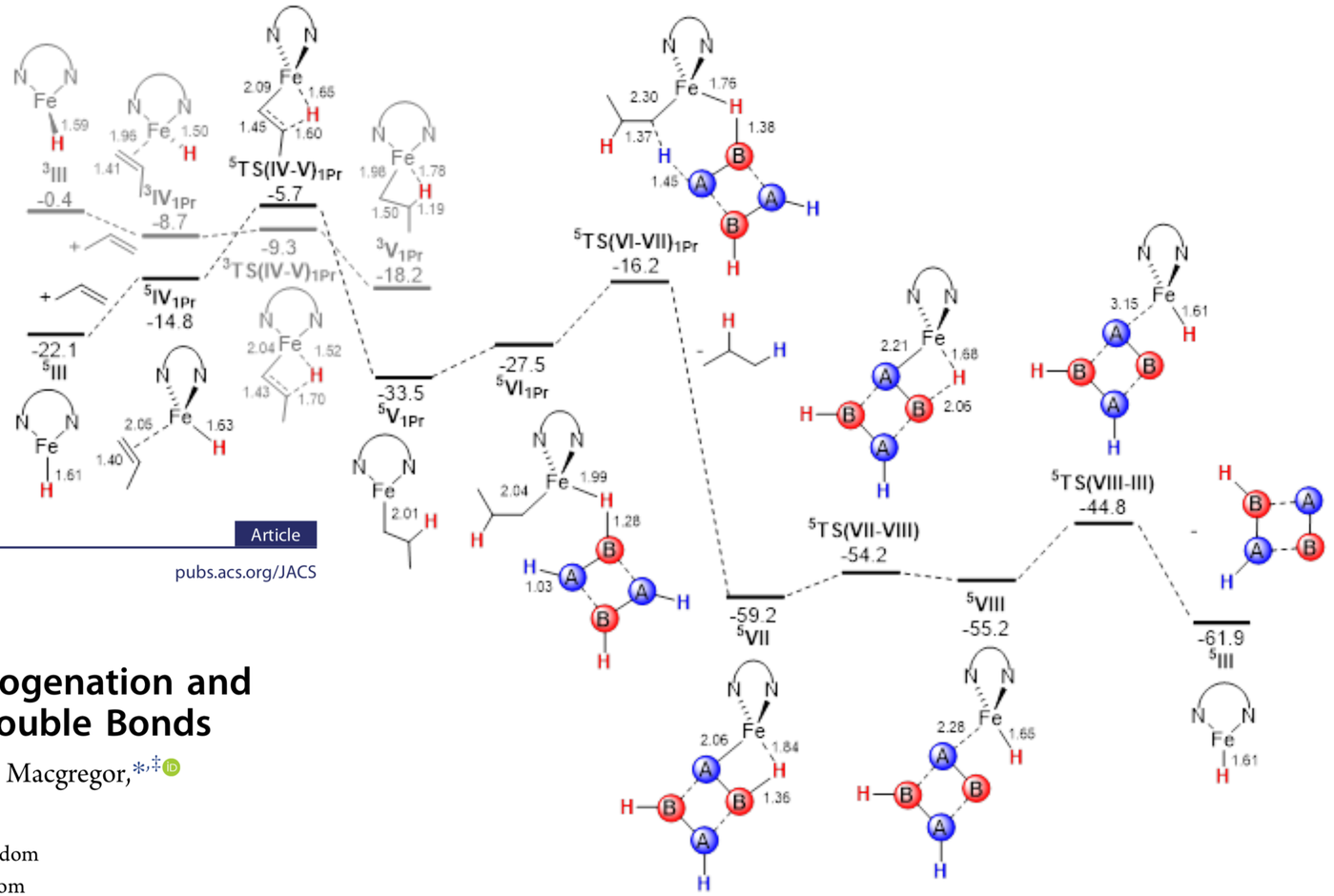


Fig. 5. Computed (DFT, B3PW91) energy profile for the reaction between compound 9 and benzene.

NOT JUST THE "COMPUTATIONAL" SECTION

- Ruth Webster



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Room Temperature Iron-Catalyzed Transfer Hydrogenation and Regioselective Deuteration of Carbon–Carbon Double Bonds

Maialen Espinal-Viguri,[†,§] Samuel E. Neale,[‡] Nathan T. Coles,[†,§] Stuart A. Macgregor,*[,‡] and Ruth L. Webster*[,†]

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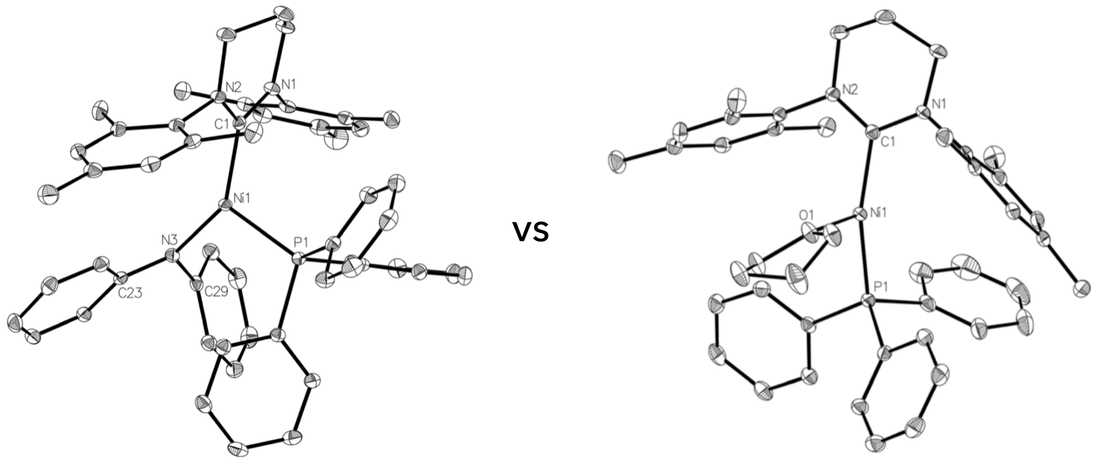
NOT JUST THE "COMPUTATIONAL" SECTION

- Mike Whittlesey, Mary Mahon (Vera Krewald)



Dalton Transactions

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Mono- and dinuclear Ni(I) products formed upon bromide abstraction from the Ni(I) ring-expanded NHC complex [Ni(6-Mes)(PPh$_3$)Br]†

William J. I
Andrea Fol
Emma Ricl
ıael J. Page,[a]
lurphy,[b]

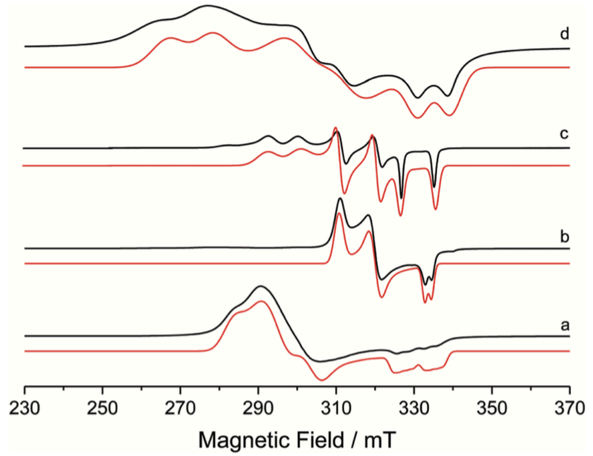
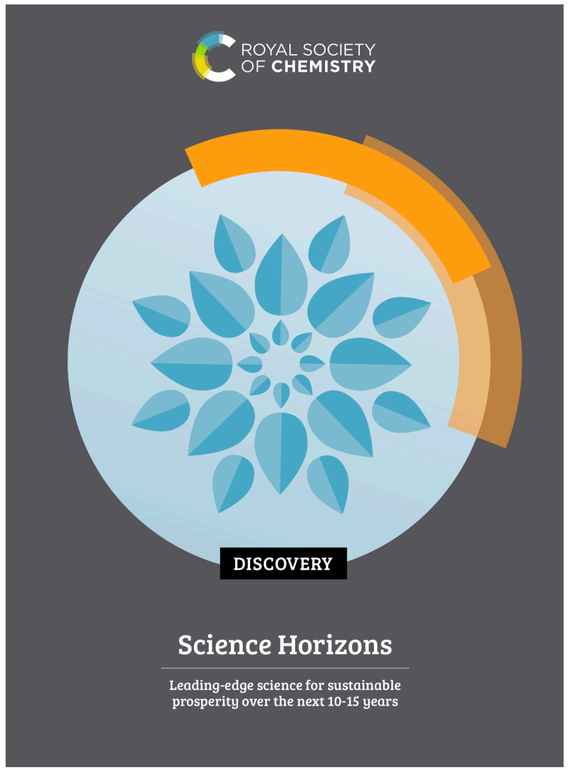
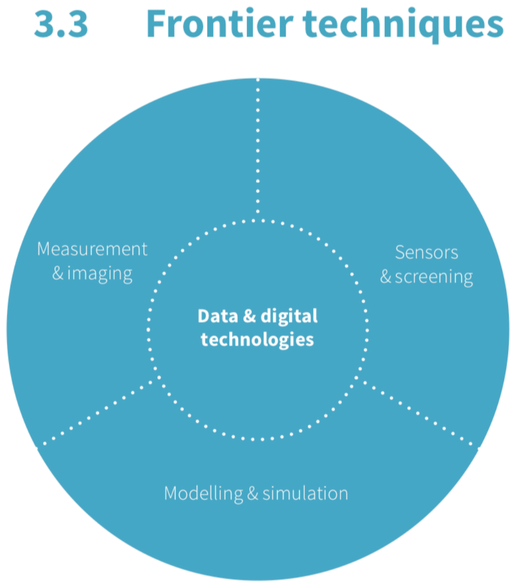


Fig. 2 Experimental (black) and simulated (red) X-band CW EPR spectra of (a) **1**, (b) **5**, (c) **8** and (d) **2** in frozen THF solution at 140 K.

COMPUTATIONAL CHEMISTRY IS EXTREMELY BROAD AND NOT JUST FOR "SPECIALISTS"

- Key area of research in the next 10–15 years.





Modelling & simulation

"Advances in theoretical and computational techniques for predicting the structure, function and properties of molecules, proteins, catalysts and materials.

Modelling & simulation is critical for the analysis and interpretation of data and for using data to make predictions and new discoveries."

COURSE PHILOSOPHY

- A "taster" of some practical computational chemistry techniques.

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- Learning by doing:
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- Learning by doing:
  - Combination of short "lectures" & hands-on programming exercises
- Why programming?
  - Have to understand what the computer is doing / not just a "black box"
  - Learn how to deconstruct a problem into an "algorithm"
  - Useful practical skill (both in chemistry and outside)

BUT I DON'T KNOW HOW TO PROGRAM!

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- We do not assume any previous programming knowledge (e.g. Y1 / Y2 labs)
  - Learning to program (using Python)
  - Solving practical chemistry problems computationally.

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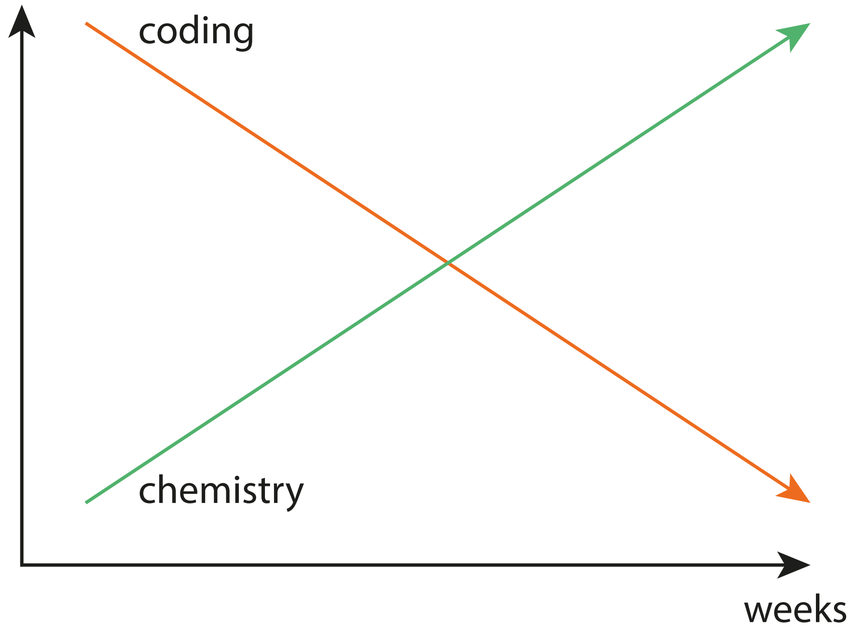

COURSE STRUCTURE

- https://moodle.bath.ac.uk/course/view.php?id=54567#section-1