COMPUTATIONAL CHEMISTRY WITH PROFESSOR JOHN KEITH

TALKING POINTS

KNOWLEDGE
1. What is a catalyst, and why is it a useful substance?
2. What is a hydride transfer?

COMPREHENSION
3. What advantages does computational chemistry have over traditional chemistry?
4. What information do John's computer models use to simulate interactions between atoms and molecules?

APPLICATION
5. Can you think of what useful end products carbon capture may produce?
6. How do you think artificial intelligence could accelerate the rate of progress of computational chemistry?
7. Why do John's findings need to be passed on to lab-based scientists rather than relying on the results of his computer models alone?

SYNTHESIS
8. John says he works with, "physicists, mechanical engineers, corrosion engineers and materials scientists". What do you think each specialist's role may be in chemical computation, and how might they interact with each other?
9. Computational chemistry is a complicated field. How would you describe it to someone with little scientific knowledge?

EVALUATION
10. John says that future computational chemists should also study humanities before using advanced technology, "to ensure that these powerful tools are being used for good." Why do you think he recommends this? To what extent do you agree and why?

ACTIVITIES YOU CAN DO AT HOME OR IN THE CLASSROOM

Catalysts have a huge array of uses, both in industry and in living organisms, and work in a number of different ways. Fill in the gaps in the following table using the internet as a research tool. Find extra examples to fill in the blank rows at the bottom.

NAME OF PROCESS	TYPE OF CATALYST	USE	HOW IT'S MADE EFFICIENT
Catalytic conversion of carbon monoxide to carbon dioxide	Platinum and other metals	Removing harmful gases from vehicle exhaust fumes	Sensors to ensure there is sufficient oxygen flow
Haber process			
	Lactase (a biological catalyst, or enzyme)		
		Washing clothes at lower temperatures	
Catalytic cracking			
		Producing sulphuric acid	

MORE RESOURCES

John Keith's website lays out the work of the Keith Lab in Computational Chemistry in researching useful catalysts:
http://www.klic.pitt.edu/

This video from the American Chemical Society explains what computational chemistry is and where it could go next:
https://www.youtube.com/watch?v=bvo7JhEMvj0

This resource presents a case study and a related worksheet on how computational chemistry provides solutions to real-world problems, in this case deterring birds from eating crops:
https://edu.rsc.org/resources/chemistry-now-computational-chemistry/55.article