

# CO<sub>2</sub> hunters!

## The CO<sub>2</sub> reduction game to learn Chemistry!

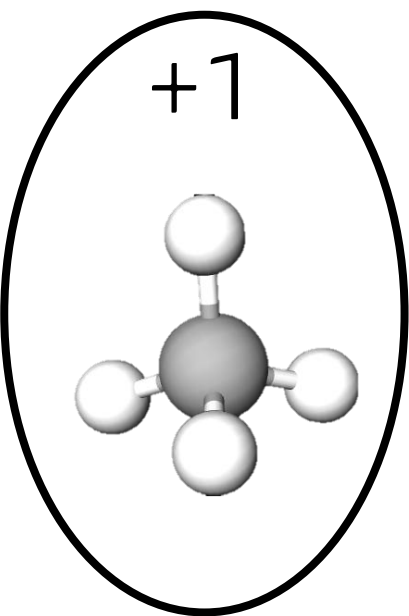
Dr. Federico Dattila  
CREST Group, DiSAT, Politecnico di Torino

Introduction to  
your research / field  
  
(to your own taste!)

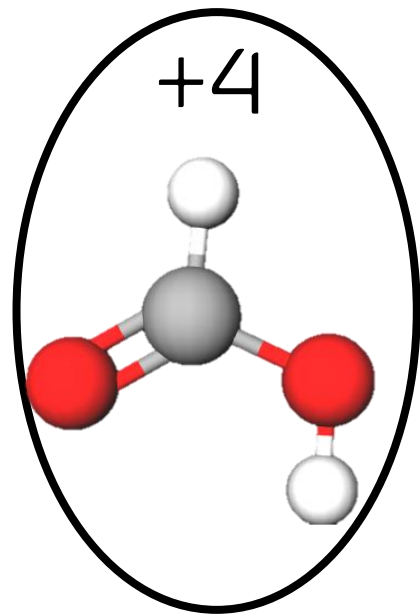
# Now it's your turn to be entrepreneurs!

1. Split into teams...
2. You have a limited time to convert  $\text{CO}_2$ ...
3. The team with best products wins!

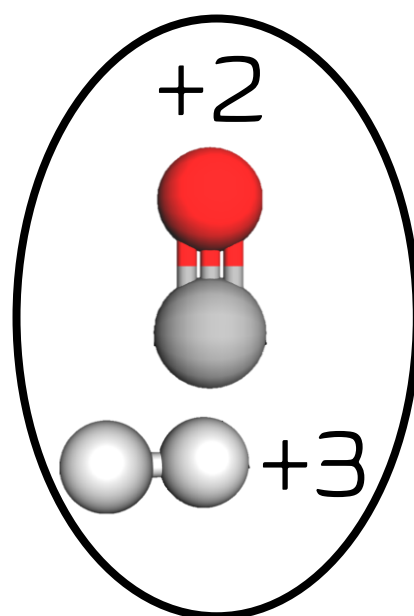
# Score



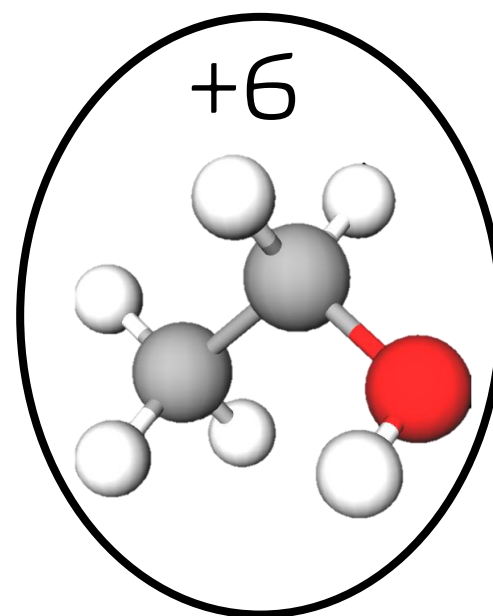
methane  
1 C, 4 H



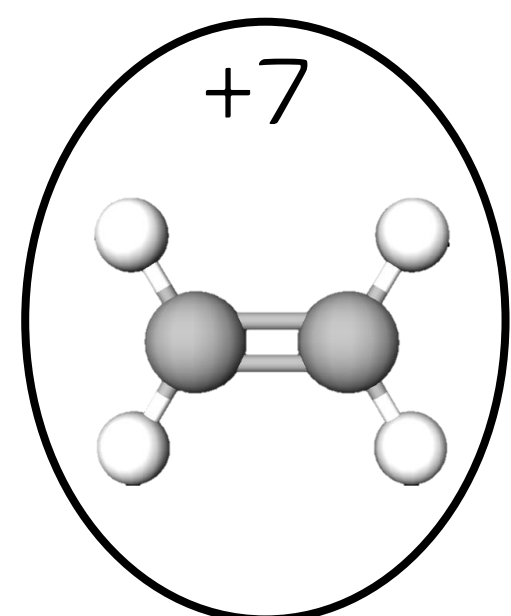
formic acid  
1 C, 2 H, 2 O



carbon monoxide  
1 C, 1 O  
hydrogen 2 H



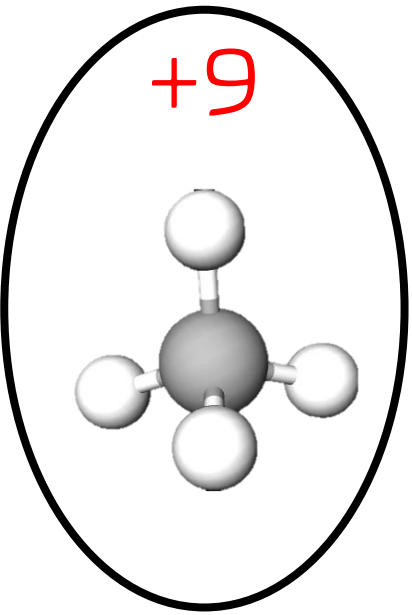
ethanol  
2 C, 6 H, 1 O



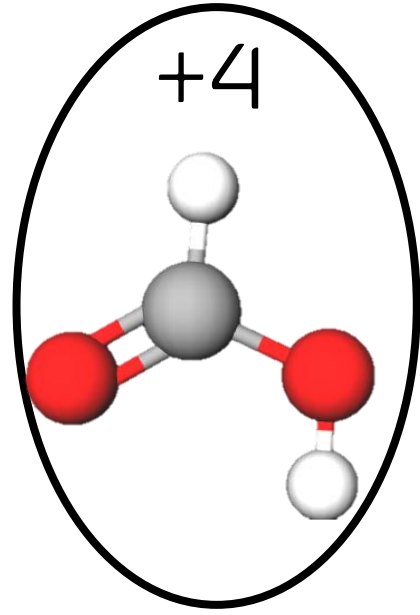
ethylene  
2 C, 4 H

Bonus: +10 if you use the most **carbon**;  
+5 if you use the most **hydrogen**.

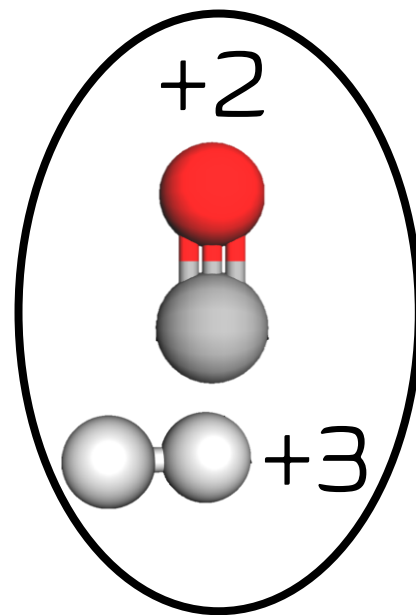
# Score (Ongoing energetic crisis!)



1 C, 4 H

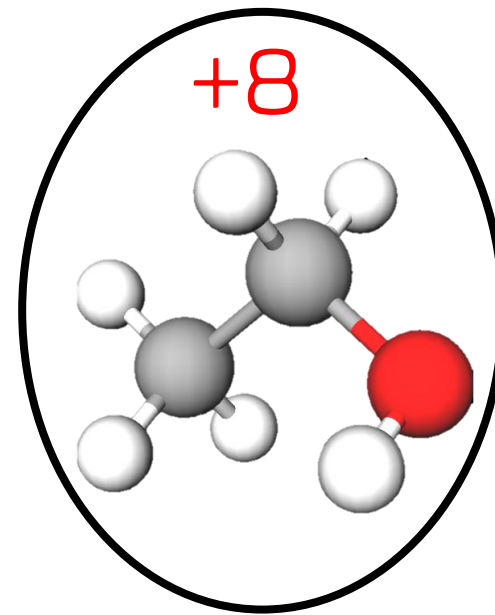


1 C, 2 H, 2 O

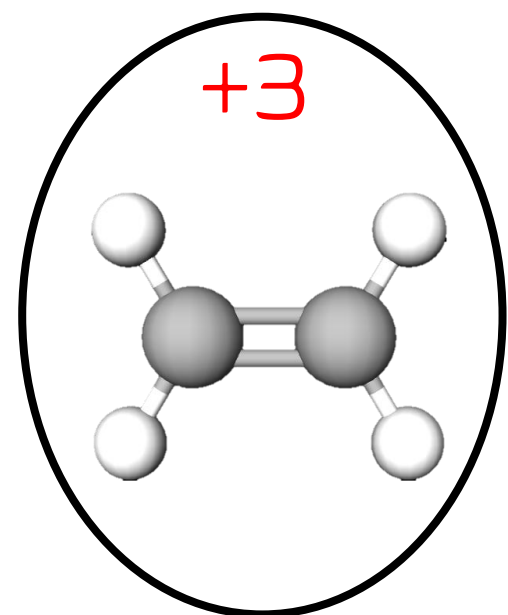


1 C, 1 O

hydrogen 2 H



2 C, 6 H, 1 O



2 C, 4 H

Bonus: +10 if you use the most **carbon**;  
+5 if you use the most **hydrogen**.

# The peer review mechanism

## CHEMICAL REVIEWS

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Review

### Modeling Operando Electrochemical CO<sub>2</sub> Reduction

Federico Dattila\*, Ranga Rohit Seemakurthi, Yecheng Zhou, and Núria López\*

Cite This: <https://doi.org/10.1021/acs.chemrev.1c00690>

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**ABSTRACT:** Since the seminal works on the application of density functional theory and the computational hydrogen electrode to electrochemical CO<sub>2</sub> reduction (eCO<sub>2</sub>R) and hydrogen evolution (HER), the modeling of both reactions has quickly evolved for the last two decades. Formulation of thermodynamic and kinetic linear scaling relationships for key intermediates on crystalline materials have led to the definition of activity volcano plots, overpotential diagrams, and full exploitation of these theoretical outcomes at laboratory



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ARTICLES

<https://doi.org/10.1038/s41929-021-00655-5>

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### Absence of CO<sub>2</sub> electroreduction on copper, gold and silver electrodes without metal cations in solution

Mariana C. O. Monteiro<sup>1</sup>, Federico Dattila<sup>2</sup>, Bellenod Hagedoorn<sup>1</sup>, Rodrigo García-Muelas<sup>2</sup>, Núria López<sup>2</sup> and Marc T. M. Koper<sup>1</sup>

The electrocatalytic reduction of carbon dioxide is widely studied for the sustainable production of fuels and chemicals. Metal ions in the electrolyte influence the reaction performance, although their main role is under discussion. Here we studied CO<sub>2</sub> reduction on gold electrodes through cyclic voltammetry and showed that, without a metal cation, the reaction does not take place in a pure 1 mM H<sub>2</sub>SO<sub>4</sub> electrolyte. We further investigated the CO<sub>2</sub> reduction with and without metal cations in solution using scanning electrochemical microscopy in the surface-generation tip-collection mode with a platinum ultramicroelectrode as a CO and H<sub>2</sub> sensor. CO is only produced on gold, silver or copper if a metal cation is added to the electrolyte. Density functional theory simulations confirmed that partially desolvated metal cations stabilize the CO<sub>2</sub><sup>-</sup> intermediate via a short-range electrostatic interaction, which enables its reduction. Overall, our results redefine the reaction mechanism and provide definitive evidence that positively charged species from the electrolyte are key to stabilize the crucial reaction intermediate.



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