CO_2 hunters!
The CO_2 reduction game to learn Chemistry!

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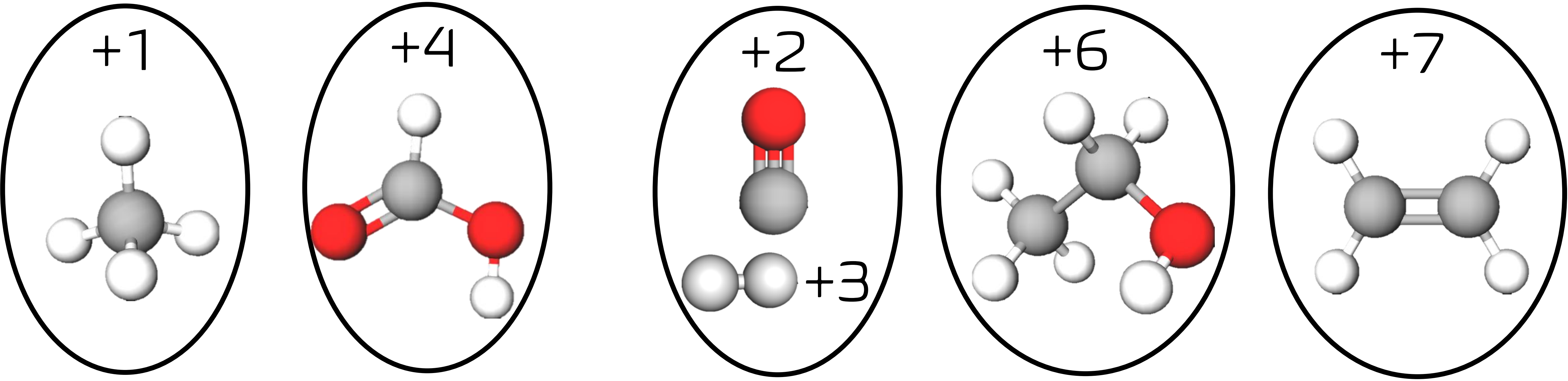
Introduction to your research / field

(to your own taste!)

Now it's your turn to be entrepreneurs!

1. Split into teams…
2. You have a limited time to convert CO_2…
3. The team with best products wins!

Score



methane
1 C, 4 H

formic acid
1 C, 2 H, 2O

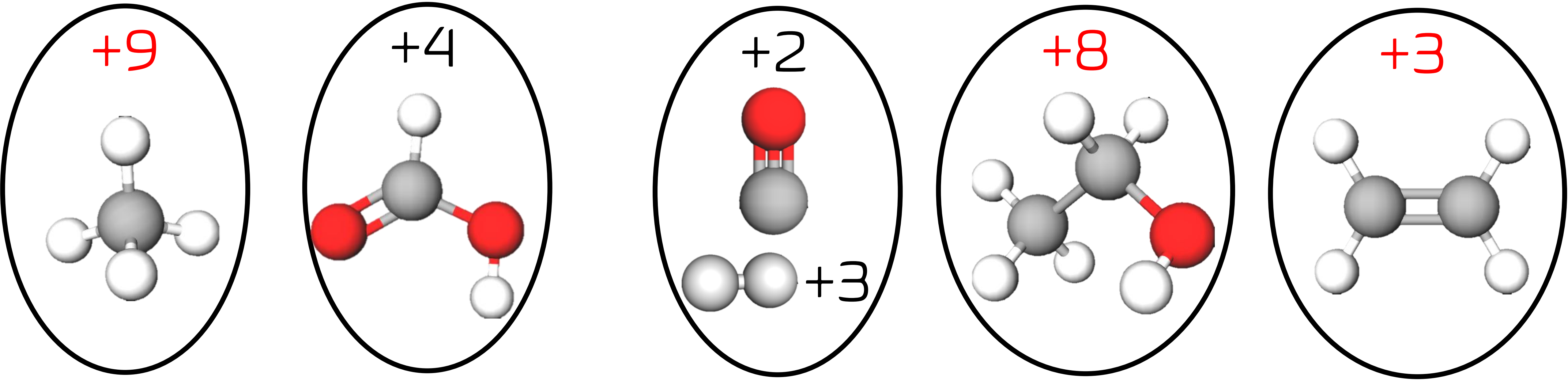
carbon monoxide
1 C, 1O
hydrogen 2H

ethanol
2 C, 6 H, 1O

ethylene
2 C, 4 H

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

Score (Ongoing energetic crisis!)



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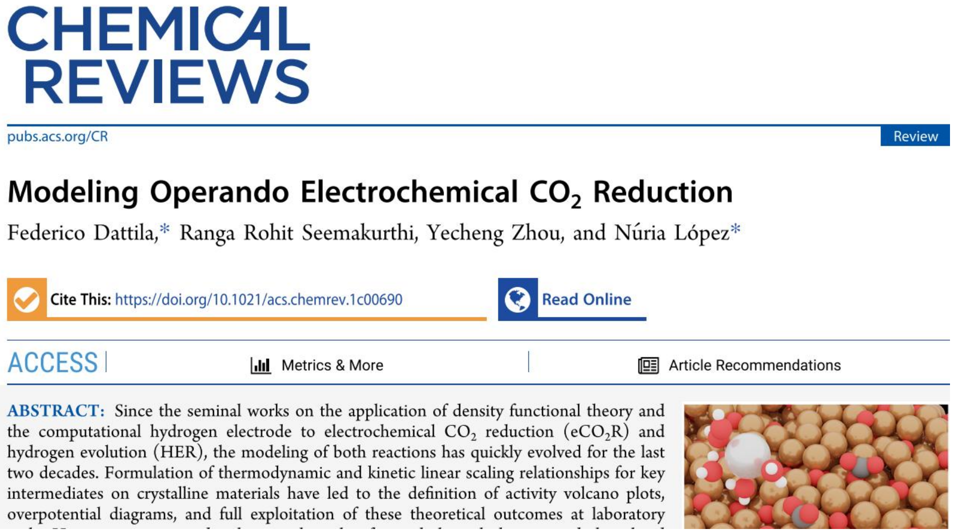
The peer review mechanism


CHEMICAL REVIEWS

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Modeling Operando Electrochemical CO_2 Reduction

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

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ABSTRACT: Since the seminal works on the application of density functional theory and the computational hydrogen electrode to electrochemical CO_2 reduction (eCO_2R) 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


nature catalysis

ARTICLES

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Absence of CO_2 electroreduction on copper, gold and silver electrodes without metal cations in solution

Mariana C. O. Monteiro[1], Federico Dattila[2], Bellenod Hagedoorn[1], Rodrigo García-Muelas[2], Núria López[2] and Marc T. M. Koper[1]

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_2 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_2SO_4 electrolyte. We further investigated the CO_2 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_2 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_2^- 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.