STUDYING HOW PLASMONS CAN DRIVE CHEMICAL REACTIONS USING HPC

MARENOSTRUM5 GPP

Led by

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1 WHAT ARE **PLASMONS** AND WHY DO THEY MATTER?

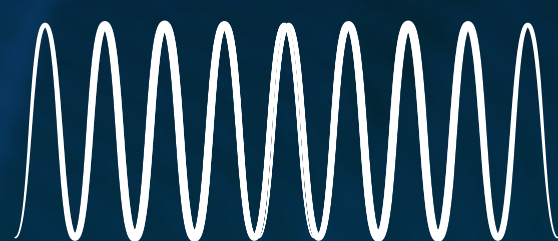
Electrons in a solid metal can **move collectively** through the material

When an **electric field** is applied, electrons shift in the **opposite direction**

Once the **field disappears**, electrostatic forces **pull the electrons back** toward their original position

However, due to their **inertia**, the electrons begin to **oscillate together**

These collective oscillations are called **plasmons**



WHY ARE THEY CRUCIAL IN CHEMICAL REACTIONS?

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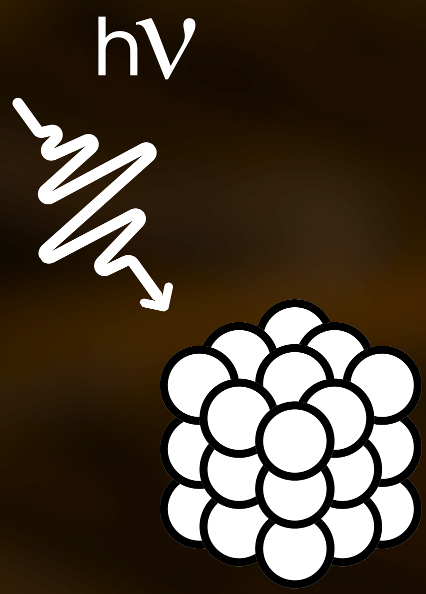


When **light hits** a metallic nanoparticle under certain conditions, **it excites these plasmons**

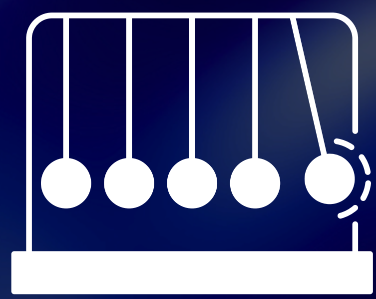
As a result, they can **strongly modify chemical reactions**, giving rise to what is known as **plasmonic catalysis**

1 → 2 → 3 → 4

Such an approach offers a promising strategy for **driving chemical transformations using light**

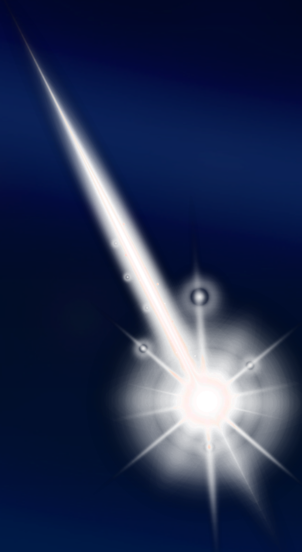
3 WHY ARE THEY DIFFICULT TO STUDY?

Researchers still struggle to identify the exact mechanism behind this phenomenon



Advanced simulations are required, but they are **extremely computationally demanding**

As a result, many studies rely on **unrealistically intense laser** fields to accelerate the process



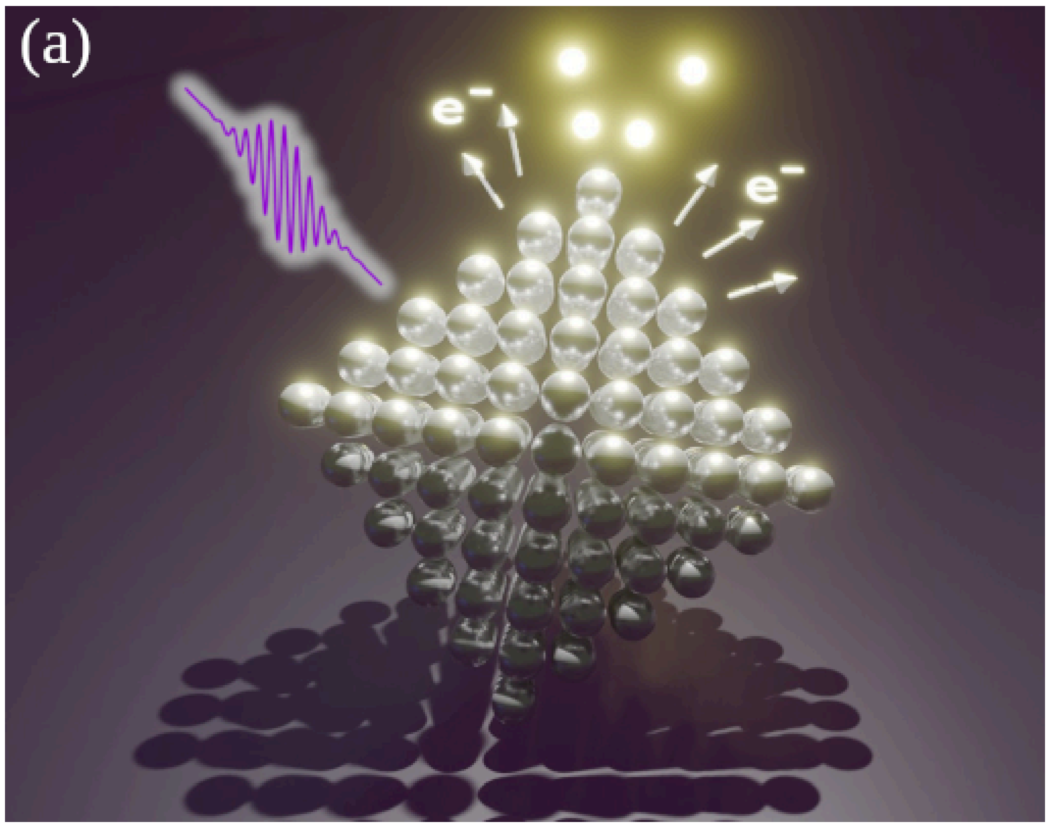
This can **mask the true plasmonic effects** observed in experiments

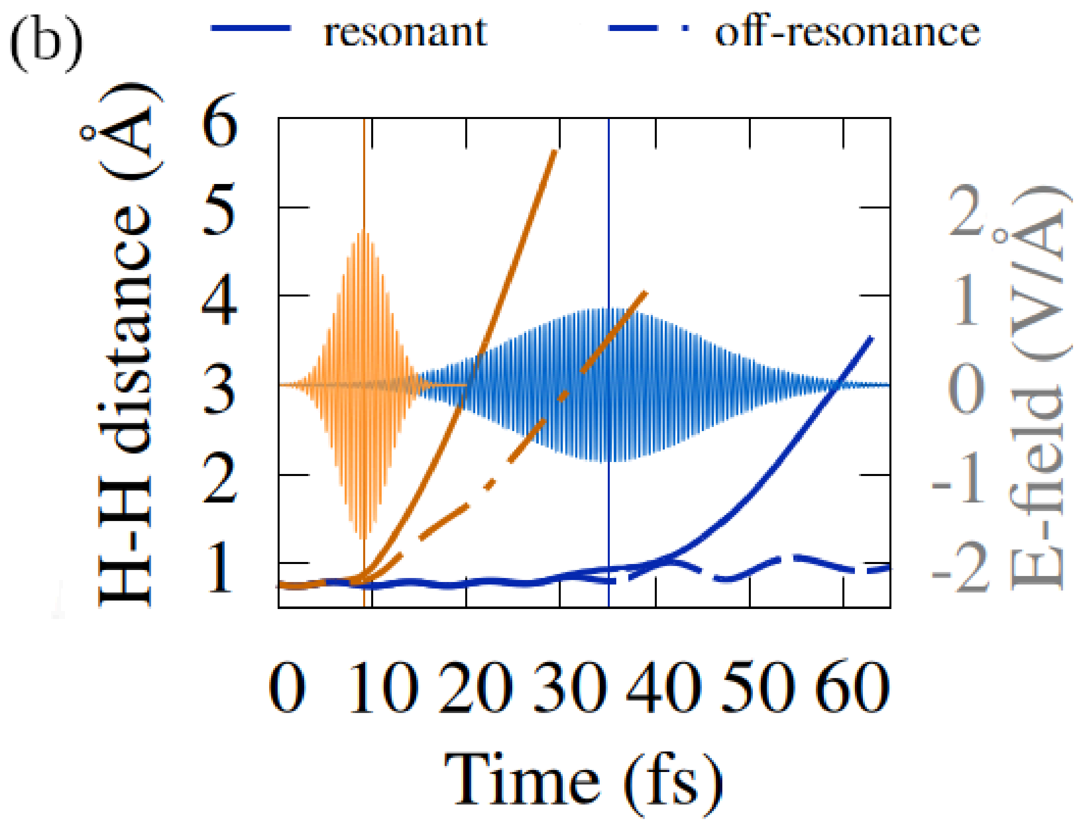
STUDYING PLASMONIC CATALYSIS WITH HPC 4

HPC enabled **longer and more realistic simulations**, reducing unwanted laser-induced effects

Under weak and long laser pulses, **reactions only occur** when the **laser frequency matches the plasmon resonance**

These results confirm that **plasmon excitation under resonant conditions drives chemical reactions**





a) Schematic illustration of **plasmon excitation in a nanoparticle by an incident photon**. Under resonant conditions, the photon excites a localized plasmon, and the effects caused are believed to play a key role in modifying and driving chemical reactions.

b) Simulation results under **short** and **long** laser pulses at resonant and off-resonance excitation frequencies. The **strong and short** laser pulse leads to H_2 dissociation at any frequency, while the **weaker and longer** pulse only does it at the plasmon frequency.