



Articles: published in [Angewandte Chemie](#) by [Juan Carlos Cuevas](#) and Linda A. Zotti, [IFIMAC](#) researchers and members of Department of Theoretical Condensed Matter Physics.

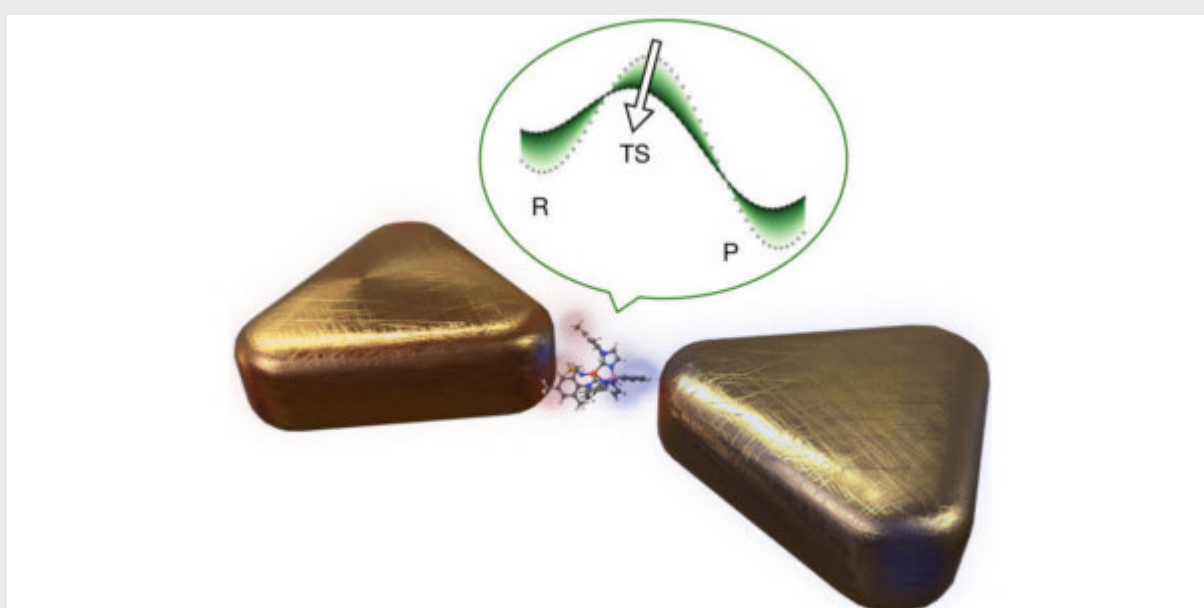
Proteins are key biological molecules that are responsible for numerous energy conversion processes such as photosynthesis or respiration. In recent years, proteins have been investigated in a new setting, namely in solid-state electronic junctions, with the goal of understanding the charge transfer mechanisms in these biomolecules, but also with the hope of developing a new generation of bio-inspired nanoscale electronic devices. Now, a new step towards this goal has been reported in a piece of work published in [Angewandte Chemie](#) by a collaboration between the group of [David Cahen](#) in the [Weizmann Institute of Science](#) (Israel) and the IFIMAC researchers Carlos Romero-Muñiz, Juan Carlos Cuevas, and Linda A. Zotti. In this work, these researchers show that a redox protein, cytochrome C, can behave as an electrically driven switch when incorporated in a solid-state junction with gold electrodes. By changing the external bias voltage in the junction, it was shown that the relevant molecular orbitals of the protein can be brought in and out of resonance with the chemical potential of the electrodes, which leads to the current-switch behavior. Showing transition from off- to on- resonance can be very challenging and this is the first time it has been achieved for proteins within the same working junction. Extensive ab initio DFT calculations revealed that the charge transport proceeds through the heme unit in these proteins and that the coupling between the protein's frontier orbitals and the electrodes is sufficiently weak to prevent Fermi level pinning. The on-off change in the electrical current was shown to persist up to room temperature, demonstrating reversible, bias-controlled switching of a protein ensemble, which provides a realistic path to protein-based

bioelectronics. [[Angewandte Chemie - full article](#)]

References

A Solid-State Protein Junction Serves as a Bias-Induced Current Switch, Jerry A. Fereiro, Ben Kayser, Carlos Romero-Muñiz, Ayelet Vilan, Dmitry A. Dolgikh, Rita V. Chertkova, Juan Carlos Cuevas, Linda A. Zotti, Israel Pecht, Mordechai Sheves, David Cahen. Published in *Angewandte Chemie International Edition*, Volume 58, Issue 34, Pages 11852-11859, August 19 (2019). [[URL](#)]

Nanocavity-modified Ground State Chemistry



Articles: published in [Angewandte Chemie](#) and [Physical Review X](#) by Javier Galego, Clàudia Climent Biescas, [Johannes Feist](#) and [Francisco J. García-Vidal](#), IFIMAC researchers and members of Department of Theoretical Condensed Matter Physics.

Over the past few years it has become clear that strong electromagnetic coupling between a molecule and light confined in a nanoscale cavity can lead to significant modifications of the electromagnetic response of the hybrid system as well as the internal molecular properties. This has already been exploited to manipulate the fate of photochemical reactions, however, up to now there has been no general theory on how these interactions affect the chemical reactivity of a molecule in its ground state without any external input of energy.

In a theoretical study published in [Physical Review X](#), a group of researchers from the [Departamento de Física Teórica de la Materia Condensada](#) and the [Condensed Matter Physics Center](#) (IFIMAC) at the [Universidad Autónoma de Madrid](#) have developed

a theoretical framework that combines quantum electrodynamics and the quantum theory of chemical reactivity. The authors implemented this approach for a simple model molecule that can be solved without approximations. This allowed to explore the general properties of cavity-induced ground-state chemical reactivity changes and develop a simplified theoretical model that can be applied to more complex molecules. They found that the induced changes on the molecular potential energy surfaces do not depend on any resonance condition between molecular transitions (such as vibrational or electronic excitations) and cavity modes, with the relevant interactions closely related to well-known electrostatic forces on the molecule due to other molecules or larger material bodies. In particular, the largest contribution to the modification of the energy landscape is typically determined by the change of the permanent dipole moment of the molecule between its equilibrium and transition state configuration. They have also shown that experimentally available nanocavities can induce changes in reaction rates by an order of magnitude in a single molecule, while for the case of many molecules, this effect becomes significant only if all the molecules are aligned.

In a second paper published in [Angewandte Chemie](#), the same authors have combined this theory with quantum chemistry calculations and have shown how plasmonic nanocavities can enable self-induced electrostatic catalysis of typical organic reactions, without any external driving, due to the interaction of the molecular permanent and fluctuating dipole moments with the plasmonic cavity modes. They have also exploited this interaction between molecules and electromagnetic modes to predict cavity-induced changes in the transition temperature of spin-crossover transition metal complexes, the prime example of molecular switches.

These studies contribute to the fundamental understanding of how nanoscale cavities can be used to manipulate chemical reactions of single molecules and open the path towards ground-state catalysis with plasmonic nanocavities. They also provide an example on how the interaction with plasmonic modes may be ultimately exploited to manipulate material properties. [[Angewandte Chemie - full article](#)] [[Physical Review X - full article](#)]
