# XLIX Congress of the Physical Chemistry Division of the Società Chimica Italiana

## Physical Chemistry: a fresh glimpse into the microscopic world

UNIVERSITÀ DI TORINO

chimica

**Torino 4-7 September 2023**

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Divisione di Chimica Fisica

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ISBN: 9788875902704



Publication date: 25-08-2023

# GENERAL INFORMATION

**Venue**

University of Turin UniTO
Dept. of Molecular Biotechnology and Health Sciences
Via Nizza 52, 10126 Torino

**Wifi**

Participants can access the wi-fi infrastructure by using the personal Eduroam account.
Please check the service has been activated on your devices.

# SOCIAL PROGRAMME

**Welcome Party**

**Monday 4 September, 2023 – h 18:30**
University of Turin UniTO
Dept. of Molecular Biotechnology and Health Sciences
Via Nizza 52, 10126 Torino

**Public Engagement**

**Tuesday 5 September, 2023 – h 18:00**
***Clima ed energia: quali scelte per il futuro?***
Cavallerizza Reale
Via Giuseppe Verdi 9, 10124 Torino

**Social Dinner**

**Wednesday 6 September, 2023 – h 20;00**
Esperia Restaurant
Corso Moncalieri 2, 10131 Torino
*(Only with reservation)*

**Techinical Secretariat**

EVENTually Meetings & Events
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# POSTERS

## T1. Physical chemistry of materials

# Zero-dimensional model for a planar Solid Oxide Electrolyser Cell (SOEC) at different working temperatures

*I. Polloni*[1*], *D. Grilli*[1], *M. Pani*[1,2], *C. Artini*[1,3], *M. Viviani*[4], *S. Presto*[4], *A. M. Asensio*[5], *A. Barbucci*[5], *P. Costamagna*[1]
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The demand for sustainable and environmentally friendly processes of producing syngas has led to the development of high-temperature co-electrolysis of carbon dioxide and steam. In an electrolyser, molecular hydrogen and oxygen are produced by water, respectively at the cathodic and anodic side, thanks to an external electrical power supply. In the same way, $CO_2$ can be converted into CO and oxygen in a reaction named carbon dioxide electrolysis. $CO_2$ and $H_2O$ electrolysis can be paired together (co-electrolysis) to obtain $H_2$ and CO, which is known as syngas, a widely used intermediate gas mixture in synthesis processes. Performing the process at high rather than low temperatures has the advantage of requiring less electrical energy. This is explained by the decrease of the ΔG of the reactions with increasing temperature[1]. Therefore, solid oxide electrolyser cells (SOECs) are currently at the cutting edge of research. Since the output syngas ratio is a key factor, it is crucial to understand the effects related to the functioning of the electrolyser. These can be estimated through a model, aiming at evaluating the current-voltage (*j*-*V*) SOEC curves and the composition of the syngas produced in different operating conditions. In this framework, a zero-dimensional model is developed. The chemical part of the model includes the calculation of the outlet cathode gas composition, considering that the water gas shift reaction occurs and reaches thermodynamic equilibrium:

$$CO + H_2O \rightleftarrows CO_2 + H_2 \quad (1)$$

The electrochemical part of the model is based on the calculation of the Nernst reversible voltage $U_N$. Then, the operating voltage U is obtained by subtracting all the voltage losses, which include ohmic, concentration and activation losses:

$$U = U_N + \eta_{ohm} + \eta_{conc} + \eta_{act} \quad (2)$$

The theoretical equations have been implemented in Matlab. The simulation results show that the $CO_2$:$H_2O$ ratio in the cathode inlet gas strongly influences the slope of the *j*-*V* curves.

This work is developed with the fundings of the National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.3 - Call for tender No. 1561 of 11.10.2022 of Ministero dell'Università e della Ricerca (MUR); funded by the European Union – NextGenerationEU- : Project code PE0000021, Concession Decree No. 1561 of 11.10.2022 adopted by Ministero dell'Università e della Ricerca (MUR), CUP - D33C22001330002, Project title "Network 4 Energy Sustainable Transition – NEST".

1. Ebbesen, S. D., Jensen, S. H., Hauch, A. & Mogensen, M. B. High Temperature Electrolysis in Alkaline Cells, Solid Proton Conducting Cells, and Solid Oxide Cells. *Chem. Rev.* **114**, 10697–10734 (2014).