REPORT ON 2nd edition of :

"CATENERCHEM : CATALYSIS-ENERGY-CHEMISTRY: Scientific and Socio-Economic Aspects of the Chemistry-Energy Nexus"

OUTLINE:

PREAMBLE: Reminder of the school objectives

In the current strive for a more renewable-energy driven society, the roadmap on catalysts development depends strongly on if and how the chemical industry can evolve to a REN-driven rather than fossil-fuel driven production. The upcoming generation of researchers in catalysis will have to be trained so as to operate the connection between the shifting techno-economic panorama of energy-related production systems and catalysis development challenges.

*"**A roadmap for catalysis to support a society powered by renewable energies**"*

This school proposes to set the basis for such an analysis, through the prism of 5 pivotal molecules that are at the roots of many current production processes:

- ***Methane:** direct conversion to methanol;*
- ***Hydrogen**: REN-production and use*
- ***Carbon dioxide**: Is "from waste to resource" building a circular economy?*
- ***Ammonia**: from fossil-based to fossil-free routes;*
- ***Polyolefin and biopolymers**: as carbon feedstock;*

These molecules are the nodes of a network with significant environmental and social consequences. The school explores this complex network, under the guide of scientists with a broad and interdisciplinary view of the field, notably with substantial contribution from social sciences.

1. ATTENDANCE

The CatEnerChem School took place in the CNRS facility « Centre Paul LANGEVIN » in Aussois (France) from March 14th to March 18th, 2022 (5 days).

98 people attended at least two days on site, with the very large majority attending three days or more on site.
The on-site attendance consisted of 73 participants (59 PhD and post-doc and 14 permanent staff), 14 speakers and 11 organizers.
16 speakers and 6 participants unable/unwilling to travel in pandemic time had access to the remote program via zoom links (broadcast program : all the main lectures, the plenary Question & Answer sessions and the practicals occurring in the main lecture hall).
In this overall 120 people-strong group, 14 countries were represented (10 EU, 4 non-EU),
F : M gender balance was about 25% in the speakers list, ca. 40% in the attendance and ca. 40 % in the organizing committee.

Figure 1. CatEnerChem 2022 group photo au Centre Paul Langevin, Aussois, taken March 15th 2022 . Unfortunately, the snow had already almost completely melted around the center, a symbol for the need for a drastic modification of our energy use.

35-H program

13h Catalysis & Chemistry
8h Social Sciences & Humanities
4h Serious Games, theater & workshops
5h Q&A+ **44 posters**
5h practicals

98 people on site

73 participants : 14 Staff + 59 PhD&PostDoc
14 speakers
11 organizers

22 remote attendants

6 participants : 4 Staff + 2 PhD
15 speakers +1 (pre-taped)

2. LECTURERS & FACILITATORS

(suffix ' *-r* ' for remote participation)

Introductory Session

Alessandra **QUADRELLI**	*CNRS & CPE Lyon*
Silvia **BORDIGA**	*UNITO & NIS*
Will **STEFFEN**-*r*	*CRI and*
William **TUMAS**-*r*	*NREL, US*

History

Antoine **MISSEMER**	*CIRED*

Economy & Psychology

Bernard **RUFFIEUX**	*U. Grenoble Alpes*
Laurence **AUFENBERG**	*Aufenberg Conseils*
Howard **KUNREUTHER** -*r*	*U PENN*

Methane

Francesco **DI RENZO**	*CNRS (Em)*
Massimo **NICOLAZZI**-r	LIMES,I
Jean-Pierre **DATH** -*r*	*TotalEnergies*
Jeroen **VAN BOKOVEN**	*ETH, CH*

Hydrogen

Vincent **ARTERO**	*CEA, CNRS, U. Grenoble Alpes*
Nathalie **DUPASSIEUX**	*CEA*
Thierry **LEPERCQ**-*r*	*Solairedirect, F*
Kylie **VINCENT**-*r*	*Oxford, UK*

CO_2

Thibault **CANTAT**	*CEA, U Paris Saclay*
J.-Christophe **PEREAU**-r	*U. Bordeaux*
Martin **SORENSEN**	*Haldor Topsoe*
Walter **LEITNER**-r	*MPG*
Andrew **BARDOW**-r	*ETHZ*

NH_3

Thoa-Minh **NGUYEN**-r	*Haldor Topsoe*
Rune **INGELS**-r	*N2Applied*
Ib **CHORKENDORFF**	*DTU, D)*

(Bio)Polymers

Elena **GROPPO**	*Unito*
Nic **FRIEDERICHS**	*SABIC*
Vincent **MONTEIL**-r	*CNRS*
Francesco **PICCHIONI**-r	*Groeningen NL*
Carlo **PEREGO**-r	*Formerly ENI*
Katalin **BARTA**-r	*U. Graz*

Scenarios& Debrief

Frédéric **CHANDEZON**	*CEA*
Bert **WECKHUYSEN**-r	*Utrecht U.*
Juliette **MICHEL**	*U Lyon*
Jindra **KRATOCHVIL**	*U Lyon*

Epistemology & Ethics

Maria-Grace **SALAMANCA**	*U. Lyon*
Paul **ANASTAS**-r	*Yale U.*

Practicals

Mathieu **PREVOT**	*CNRS*
Bertrand **REUILLARD**	*CEA, CNRS, U. Grenoble Alpes*
Matteo **SIGNORILE**	*UNITO*
Manoja **RAVI**-r	*U. Birmingham*
Xavier **CARRIER**	*Sorbonne U*

3. ANALYSIS OF THE SCIENTIFIC OUTCOME

The most original feature of the 5-day thematic school was its resolutely trans-disciplinary content (see outline program in figure 1, and detailed program attached to this report) that matched, or even superseded, the initially planned content.

The transdisciplinary week content was articulated around different types of interventions :

- general courses on the energy transition, its broad framework (anthropocene) - dark green code in figure 1.

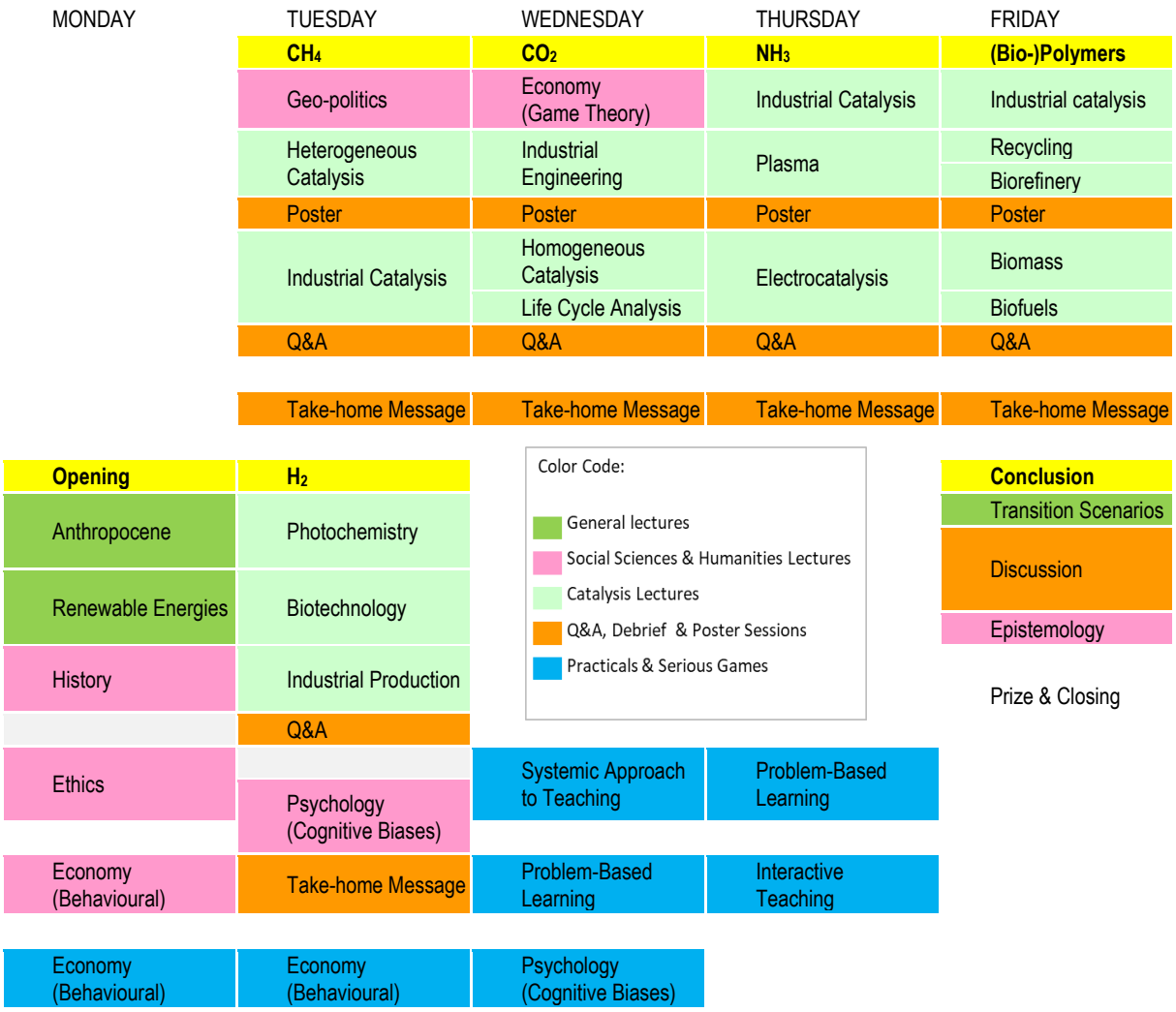
- lectures on exemplary research in catalysis of transformation of molecules at the heart of the energy transition (methane, hydrogen, carbon dioxide, ammonia and (bio)polymers) by highlighting various fields (heterogeneous catalysis, enzymatic, industrial, photochemistry, electrochemistry, recycling of polymers, life cycle analysis, synthesis of biofuels, transformation of biomass) -green code in figure 1.

- courses in the humanities and social sciences (history, geopolitics, psychology, ethics, economics) and the links with the scientific method adapted to this systemic context (epistemology) that shed light on the issues at stake in the theme -pink code in figure 1.

- practical and serious games that proposed pedagogically innovative ways to teach adapted to systemic nature of sustainability issues (Systemic approach to learning, problem based learning, interactive instant olling teaching, serious games on cognitive biases, theater atelier for ethics in science)- blue code in figure 1.

- participant-led events (long Q&A sessions with speakers, debrief "take-home message" sessions only among participants)- orange code in figure 1.

Figure 1: Outline of CatEnerChem Final program



The hybrid mode, which was decided six weeks before the starting date due to the pandemic situation, allowed to substantially increase the number and diversify the geographic origin of speakers giving a mix of in presence speakers and organizers (22 people, in depth 30' lectures) with short and very focused interventions (21 speakers, 15' lecture), for a final roster of lectures, see section below "2022 Lecturers & Facilitators", that surpassed our initially planned all presence program (excellent yet more modest for obvious financial and logistic reasons).

As a thematic school, CatEnerChem offers some insightful lesson from the viewpoint of evaluating its scientific validity :

1. **The link between chemistry and the broad framework of the Anthropocene** (the topic of the CatEnerChem opening course by W. Steffen a forefather of the planetary limit concept) is strong and provides a relevant framework for complex systemic analysis of the energy-chemistry nexus (as evidenced by recent papers such as Stephen A. Matlin, Sarah E. Cornell, Alain Krief, Henning Hopf and Goverdhan Mehta "*Chemistry must respond to the crisis of transgression of planetary boundaries*" **Chem. Sci**. 2022, 13, 11710).

2. The importance of **embedding advances in a specific research topic** (e.g. chemical use of CO_2, defossilized production of NH_3) in **a broad understanding of the underpinning cycle** (carbon cycle, nitrogen cycle) and the underlying planetary boundaries This approach too can be found in the leading literature M. Whalen, S. A. Matlin, T. A. Holme, J. J. Stewart, and P G. Mahaffy* "*A Systems Approach to Chemistry Is Required to Achieve Sustainable Transformation of Matter: The Case of Ammonia and Reactive Nitrogen*" **ACS Sustainable Chem. Eng**. 2022, 10, 39, 12933-12947

3. The relevance of concepts from philosophy, epistemology, history, geography and other SHS disciplines to understand and **overcome the disciplinary compartmentalization and reductionist approach** that still runs through our field and that are little in line with the systemic and complex nature of the changes underway.

4. ANALYSIS OF THE PEDAGOGIC OUTCOME

The pedagogical objectives of the school were achieved
- The diverse program trained the participants in the execution, the analysis and the reflexivity around research in catalysis (thermal and otherwise assisted - photo, electro, ...)

-The power of **new learning methods** (e.g. theater-based workshops on ethics, interactive practicals through instant polling, debriefing sessions, video recording of self-reflexive considerations, practicals based on systemic approaches, serious games in psychology, long Question&Answer sessions, …) that reflect the systemic, demanding, reflective and decentered nature that the Anthropocene requires

- The content of the collective analysis discussions at the end of each session showed the relevance of a transdisciplinary approach - to grasp the transdisciplinary chain of knowledge that the program has systematically explored:
    - Elements of the systemic environmental, socio-economic and ethical context of the field
    - Current state of the art of the industrial production in chemistry of five "pivotal" molecules
    - Identification of catalytic solutions currently at work and being improved for each one
    - Tools (epistemological, among others) for the reflexive analysis of the scenarios that these solutions imply, for example, the work via "serious games" for an awareness-raising work on the cognitive barriers to be taken into account in order to favor the energy transition
    - Impulse of a multidisciplinary reflection group, made up of a group of about twenty people having attended the school (speakers and participants) which gathers permanent staff, post docs and doctoral students from several countries, with a chemical barycenter and profiles from the SHS (history, economics, philosophy, geography) around the proposed approach (a face-to-face meeting on June 1-3, 2022 in Lyon and 3 meetings in distance from the school, in view of the co-writing of a collective "perspective article" on the subject

5. FINANCIAL REPORT

The budget of the school is at equilibrium (see Table 2).
The lower than forecasted revenue (84,50 k€ effective vs. 102 k€ forecasted) have been for ca. 1/3 from registrations and ca 2/3 form sponsorship.

The main missing source of revenue was from the presence of 79 participants rather than the forecasted 100. This said, given the pandemic situation, we consider the presence of 79 participants a success.

Among the 79 participants, 49 people (62%) benefited of at least partial fees waving (waiver ranging from 150 EUR/person to 650 EUR/person, with respect of a full fee of 650 EUR/person which covers pedagogic content, lodging and meals throughout the week). Details of fee waivers are available in Table 2.

The logos of the sponsors and media partners are reported in Figure 2:

Figure 2: Logos of sponsors and media partners of CatEnerChem 2022

The expenses (84.50 k€) were less than the forecasted (102 k€) mostly because of the lower than predicted registrations. A further and unanticipated serious expenditure was that all the registration fees and international sponsorship (EFCATS, GIC-SCI, and INSTM) were subject to 20% VAT (for example, when a participant paid 650 EUR, the school registrations amounted *de facto* to 541.67 EUR in the budget). In view of the negative forecast all non-core preparatory expenses (e.g. USB keys, hardcopy printouts, paper communication, …) were abandoned. The pandemic-induced decision to offer remote participation option to the speakers, as well as the generous decision of several on-site speakers and organizers not to request reimbursement allowed to reduce expenses. The major factor that allowed to stay within budget was that the hosting facilities, Centre Paul Langevin in Aussois (F), billed based on effective presence and with daily precision and not on forecasted attendance and bulk billing by the week even for shorter stays. Due to this unexpected (and frankly unhoped for) financial latitude the private school CPE school was reimbursed of ca. 50% of its indirect costs connected to organizing the school (accounting and secretariat mostly). A debriefing meeting was organized in Lyon in July among all the participants that were interested in participating in a collective perspective article; this action and further ones around valorizing the school content are ongoing (see perspective section).

Table 2: CatEnerChem 2022 Budget

Note: this budget incorporates the registration reductions from the bursary grants directly in the revenues, and not anymore in section (4) of expenditures, as was the case for the provisional budget,

for French transactions	VAT-free	*forecasted in provisional budget*
Revenues : (1) + (2) En K€	**84,50**	***(forectasted: 111,03 -9 k€)***
(1) Registration fees	**31,60**	*(forecasted: 43= 52 k€- 9k€)*
30 full-fee participants (650 €/pers)	19,50	
16 fully-waived fee bursary grants (fees paid by ET CNRS grant)	0,00	
25 PhDbursary grants (250 EUR ea.=> registration becomes 400 EUR)	10,00	
3 full-Permanent researcher bursary grants (200 EUR ea. => registration becomes 450 EUR)	1,35	
5 GIC-SCI PhD bursary grants (500 EUR ea.=> registration becomes 150 EUR)	0,75	
14 on -site Speakers (registrations waived)	0,00	
14 on-site Organizers (registrations waived)	0,00	
18 remote speakers	0,00	
(2) Sponsorship & Media PARTENER	**52,90**	*(forecasted: 59 k€)*
LABEX Arcane	2,00	
GDR solar Fuels	4,00	
ET CNRS	13,00	
LABEX CHARMMMAT	2,50	
EUL	10,00	
CEA	3,00	
IRCELYON	3,00	
EFCATS	10,00	
GIC -SCI	2,50	
INSTM	2,00	
ICL	0,50	
RSC	0,40	
SCF RA	0,00	
EUCHEMS	0,00	
Expenditures : (1) + (2) + (3) + (5) + (6) En K€	**84,50**	***(forectasted: 111,03- 9 k€)***
(1) Logistics on site	**43,64**	*(forecasted: 78,26 k€)*
Travel onsite speakers + on-site organizers	1,02	*(forecasted: 8 k€)*
Frais de séjour (45€/nuit/Personne* 91) 4 nuits	35,37	*(forecasted: 58,96 k€)*
Bus shuttle participants	0,84	*(forecasted: 1,5 k€)*
Auditorium rent (24 EUR/PAX)	2,65	*(forecasted: 3 k€)*
social dinner (@41,5 EUR ea)	3,36	*(forecasted: 5,7 k€)*
Prizes for particpants by RSC (best visual summary, best poster(s), best attendant)	0,40	*(forecasted: 1 k€)*
(2) Hand-outs to participants et Communication ahead of event	**8,62**	*(forecasted: 8,5 k€)*
Prints + postage (2 rounds of flyer + posters pdf)	0,00	*(forecasted: 1,5 k€)*
Postage	0,00	*(forecasted: 0,5 k€)*
USB keys for participants	0,00	*(forecasted: 1 k€)*
Hard copy pedagogic content + abstract in 100 copies	0,00	*(forecasted: 3 k€)*
Externalization Psycho + Economy courses	1,08	*(forecasted: 0 k€)*
web site (creation site, hosting 2021, 2022)	5,04	*(forecasted: 1 k€)*
CPE communication services	2,50	*(forecasted: 1,5 k€)*
(3) Accounting and Secrétariat	**13,79**	*(forecasted: 9 k€)*
accounting services & management CPE (handling registrations and billing)	6,00	*(forecasted: 3 k€)*
temporary assistance secreteriat : missions: follow up on funding applications, registration, follow up	7,20	*(forecasted: 6 k€)*
off site consortium meeting expenses (e.g. preparatory meetings, office supplies)	0,59	
(4) Bursary Grants (SCF, SCI, EFCATS,)	now in revenues (9.35)	*(forecasted: 9 k€)*
25 PhD (non CNRS) bursary grants (250 EUR ea.=> registration becomes 400 EUR)	(see revenues)	
3 full-Permanent researcher bursary grants (200 EUR ea. => registration becomes 450 EUR)	(see revenues)	
5 GIC-SCI PhD (non CNRS) bursary grants (500 EUR ea.=> registration becomes 150 EUR	(see revenues)	
16 CNRS fully paid particpants (fee waived in forecast revenue section)	(see revenues)	
(5) Output	**10,76**	*(forecasted: 6.5 k€)*
2-person team recording and broadcasting on site during 5 days	2,02	
transcript (collective paper open access)	2,00	
de-briefing meeting 1st -3rd /06/2022 common paper	3,22	
hebergement site 2023-2024 and site revamp	2,02	
output production (video archiving) -ongoing	1,50	
(6) VAT taxes on revenue	**7,68**	*(forecasted: 0 k€)*
taxes on all iinternatinal registration fees and VAT-free sponsorships (SCI, EFCATS, INSTM)	7,68	*(forecasted: 0 k€)*
BILAN : (Expenditures- Revenue) en K€	**0,00**	

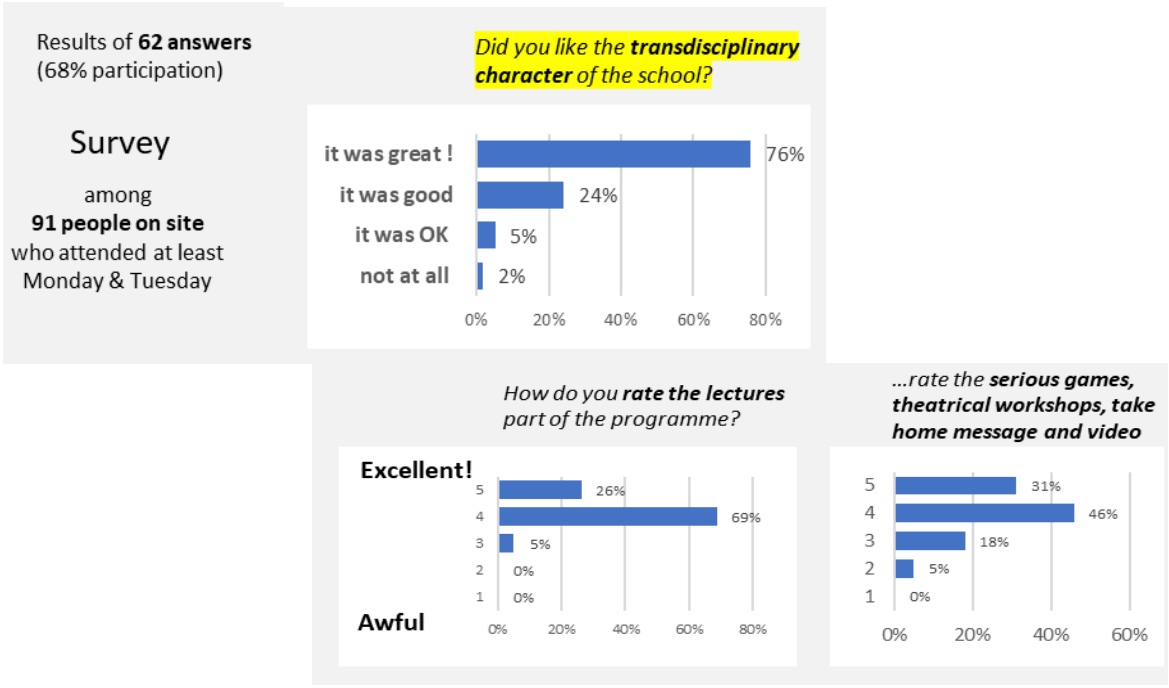
6. SURVEY RESULTS

6-a) Scientific aspects

Positive points:

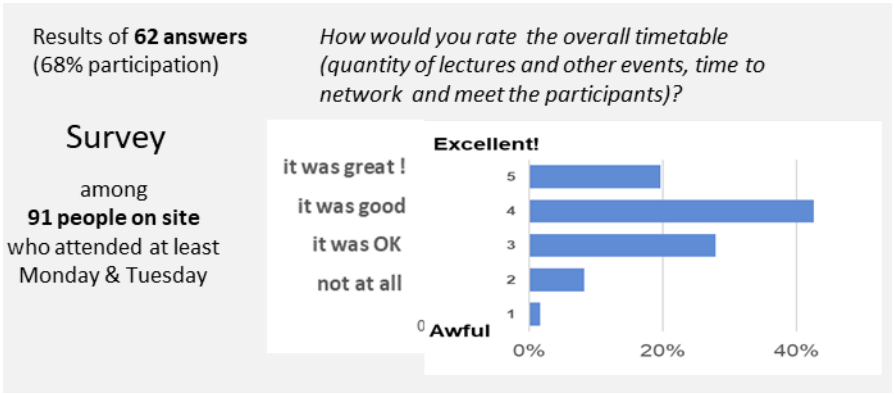
- The program articulated around 5 molecules and their respective cycles allows to grasp and cross several major issues of the subject while offering a comprehensible framework that was appreciated

- The contributions of the SHS courses (history, economy, earth system sciences, psychology, epistemology) , build notably through the strong scientific and pedagogic support of école urbaine, and the modes of pedagogy other than the "classic" presentation with a face-to-face teacher (other modes: serious games in psychology, theater workshops for ethics, long Question&Answer sessions, exchange workshops,...) allowed to achieve the objectives and were very appreciated by the participants

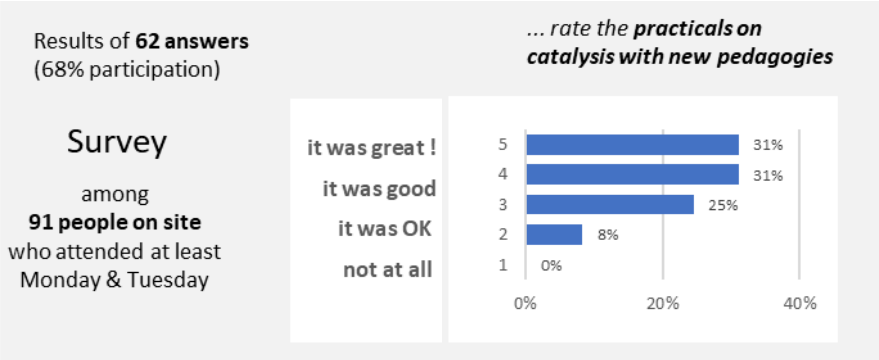


Points to be improved:

- Inability for the moment to attract participants from the SHS (see list of participants) despite considerable effort. Find other relays to circulate the information
- the program was appreciated (see survey) but by analyzing the comments (not shown here) too dense at times with too short poster sessions (proposal: reduce to 2 or 3 pivotal molecules and organize the program around these)



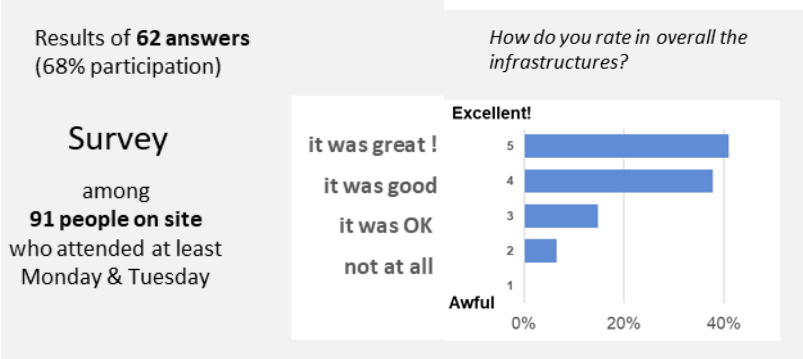
- While the remote lectures did not lose their verve because of the hybrid mode (the practicals with new pedagogies, which is still an interesting trial balloon, and the late afternoon end of the week schedule suffered more form the hybrid mode), see survey below:



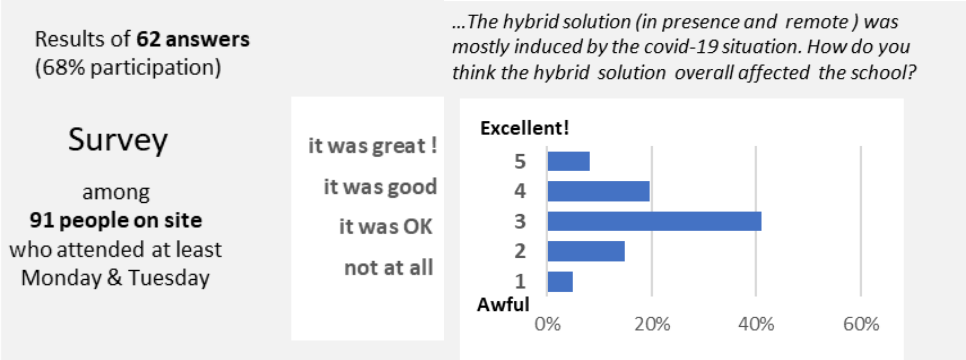
6-b) Organizational aspects

Positive points

- The infrastructures were globally appreciated:



- the hybrid formula (participants & organizers mainly in person and speakers mainly in remote) imposed by the pandemic and relatively appreciated by the participants



In our opinion, on the contrary, the hybrid formula worked beyond expectations: technically, thanks to the invaluable technical support of the urban school's audiovisual team, but also because in our opinion, the hybrid formula unlocked some potentially blocking points. Three outstanding examples:

o 1. ability to involve prestigious speakers initially not involved because of costs (see. Final live video conference of Paul Anastas, founder of the Green Chemistry Principles and Volvo Environmental Prize 2022) and to be able to ask for short and punchy interventions (15-20 min) that cannot be asked to someone who has made the trip. Possibility of crossing several points of view - more interventions than initially planned

o 2. Creation of a group cohesion on site allowing an advanced and independent analysis of the proposed contents

o 3. Invoicing as close as possible to the real situation (nights and meals actually used invoiced independently of the estimate, even for partial stays) is particularly important in the period of the pandemic

(unexpected absences, many uncertainties) and has greatly improved the financial balance of the school, which, in view of the tax system of CPE FCR (the school's managing body, therefore subject to VAT), and the pandemic could have been disastrous (for financial section above)

Areas for improvement:

- The restoration of the Paul Langevin did not fully convince, as was evident from the comments related to the 'infrastructure' survey question shown above.

7. PERSPECTIVE

The co-authoring of a collective "perspective article" on the topic by a group that participated in the school and chose to continue working together during the closing session of the school (see photo) is underway

Fig. 3: School's closing debriefing, Friday, March 18, starting point of the collective writing work in progress.

The choice of the exploitation mode of the audio and video material during the school is under evaluation (for the moment each participant has access to the recorded courses and the supports on a dedicated site).
A third 2024 Edition is envisaged and it would be chaired by Prof. Silvia Bordiga, and co -chaired by Dr. A. Quadrelli.

Reminder of the 2022 edition school bodies

CONFERENCE CHAIR

Alessandra **QUADRELLI** *Chair* CNRS* CPE Lyon

Silvia **BORDIGA** *Co-chair* U. Torino NIS*

*CNRS Centre National de la Recherche Scientifique

*NIS Centre for nanostructured interfaces and surfaces

SCIENTIFIC BOARD

Vincent ARTERO (CEA); Clément CAMP (CNRS) ; Thibault CANTAT (CEA) ; Sophie CARENCO (CNRS) ; Francesco DI RENZO (SNRS); François JEROME (CNRS); Mathieu PREVOT (CNRS) ; Bertrand Reuillard (CEA) ; Isabelle VIO (EUL, Université de Lyon).

CPE ORGANIZING COMMITTEE

Emmanuelel Almendra (communication), Florence Terraz , now Emilie Giroud (accounting) , Clémence Nikitine, Gérard. Pignault (direction), Alessandra Quadrelli (chair)