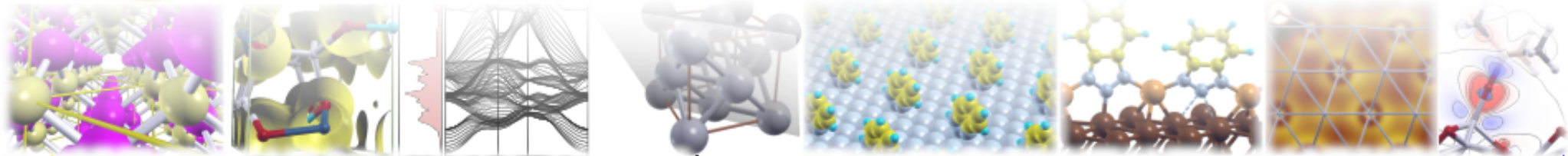




QUANTUMESPRESSO

September 15–20, 2019
Ljubljana, Slovenia

Summer School on Advanced Materials and Molecular Modelling




WELCOME



QUANTUM ESPRESSO
FOUNDATION

MAX DRIVING
THE EXASCALE
TRANSITION

 Jožef Stefan
Institute
Ljubljana, Slovenija

 **cecam**
Centre Européen de Calcul Atomique et Moléculaire

 **EUROTECH**
Imagine. Build. Succeed.

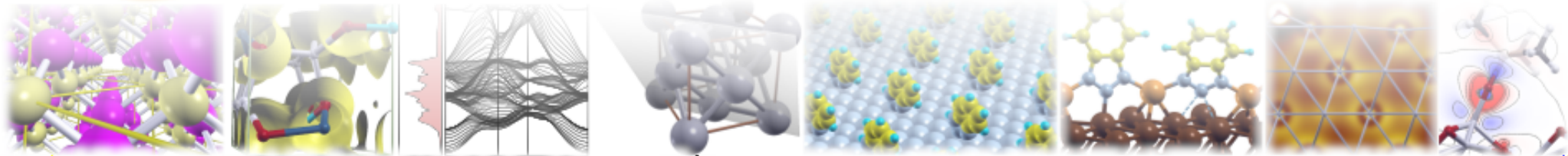


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Opening remarks & general instructions



QUANTUM ESPRESSO
FOUNDATION

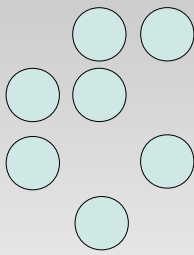
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About QE-2019



▼ Organizers

Stefano Baroni (SISSA, Trieste)

Anton Kokalj (Jožef Stefan Institute, Ljubljana)

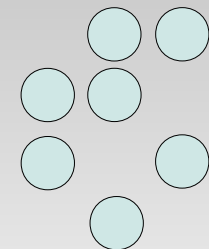
Ivor Lončarić (Ruđer Bošković Institute, Zagreb)

Antun Balaž (Institute of Physics Belgrade)

▼ School Motivation

The aim of the Summer School is to introduce students, postdocs, and other researchers to materials and molecular modelling with QUANTUM ESPRESSO. The school covers basic concepts as well as recent advances and developments, with emphasis on density-functional-theory based methods and high-performance computing ...

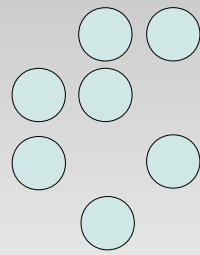
Acknowledgments



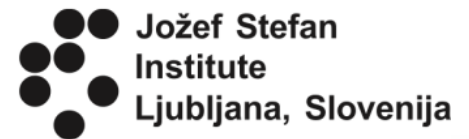
- ▼ A special acknowledgment goes to:
 - ▼ **lecturers and tutors**
 - ▼ **Matic Poberžnik** (organization & logistics, implementation of school virtual-machine),
 - ▼ **Matjaž Dlouhy** (organization & logistics),
 - ▼ **Jan Jona Javoršek** and **Barbara Krašovec** (for support concerning HPC facilities),
 - ▼ **Barbara Kapun, Dolores Zimerl, Tatjana Močnik, and Francesca Garofalo** (administration),
 - ▼ **Networking Infrastructure Centre (CMI)** for making the HPC facilities available for the school,
 - ▼ **Department of Knowledge Technologies (E8)** and **Department of Communication Systems (E6)** for making their video-classroom available for the school,
- ▼ and all others who contributed.
- ▼ Help from personnel of the **Department of Physical and Organic Chemistry** at Jožef Stefan Institute is much appreciated and acknowledged.

Apology to those who I forgot to mention ...

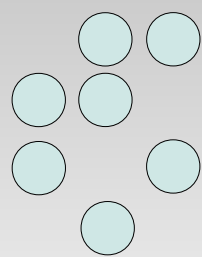
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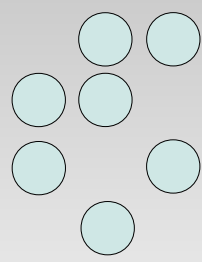
Sponsors



About Jožef Stefan Institute



About Jožef Stefan Institute



Stefan-Boltzmann Law

$$E = \sigma T^4$$

USE °K

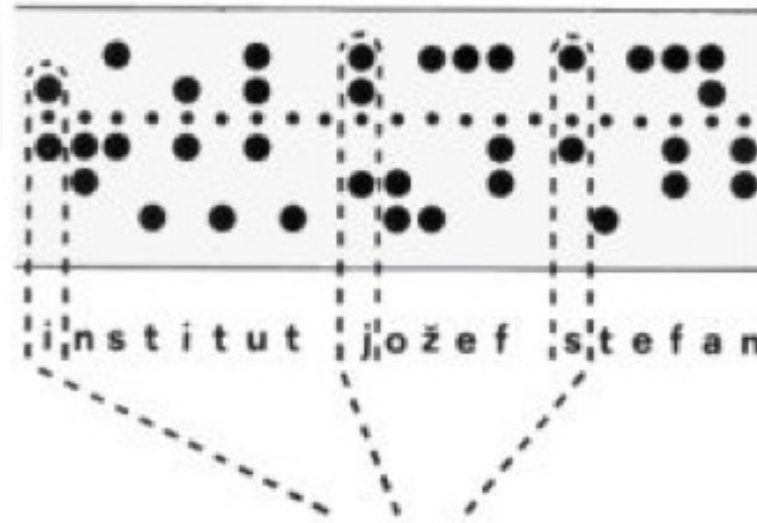
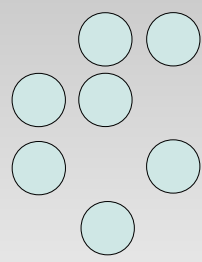
A small increase in temperature causes a big increase in emitted energy



The Jožef Stefan Institute is named after the distinguished 19th century physicist Jožef Stefan, most famous for his work on the Stefan-Boltzmann law of black-body radiation.

- leading research organization in Slovenia
- founded in 1949 as Institute of Physics within the Slovenian Academy of Sciences and Art
- the staff of more than 960 (≈450 PhDs and 200 PhD students) specializes in natural sciences, life sciences and engineering.

About Jožef Stefan Institute



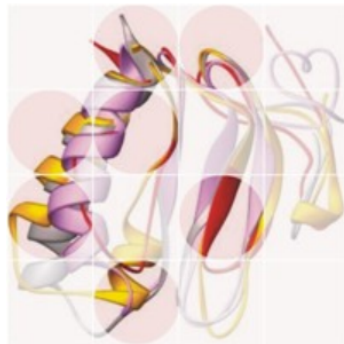
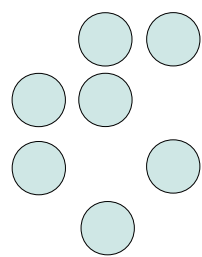
$$j = \sigma T^4$$

$$j = \text{⋯} T^4$$



=





In terms of research the Institute is divided into departments, laboratories and centres. The departments perform the research activity that is defined as a long-term programme of the Institute. In order to pursue the programme of the research, educational and other expert activities the work of the departments is coordinated within the context of the broader activity of the Institute.

The Institute pursues its activity by engaging in research programmes, research projects, development programmes and projects for the establishment and maintenance of the research infrastructure.

RESEARCH DEPARTMENTS

Physics

Theoretical Physics F1
Low and Medium Energy Physics F2
Thin Films and Surfaces F3
Surface Engineering and Optoelectronics F4
Condensed Matter Physics F5
Complex Matter F7
Reactor Physics F8
Experimental Particle Physics F9

Chemistry and Biochemistry

Biochemistry and Molecular Biology B1
Molecular and Biomedical Sciences B2
Biotechnology B3
Inorganic Chemistry and Technology K1
Physical and Organic Chemistry K3
Electronic Ceramics K5
Nanostructured Materials K7
Synthesis of Materials K8
Advanced Materials K9
Environmental Sciences O2

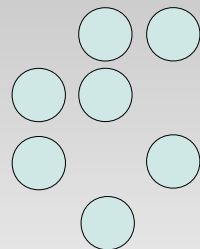
Electronics and Information Technologies

Automation, Biocybernetics and Robotics E1
Systems and Control E2
Artificial Intelligence E3
Open Computer Systems and Networks E5
Communication Systems E6
Computer Systems E7
Knowledge Technologies E8
Intelligent Systems E9

Reactor Engineering and Energetics

Reactor Engineering R4

About K3 Department



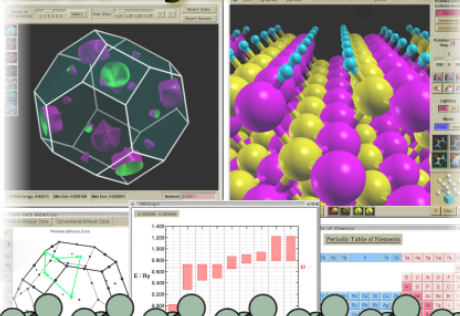
K3: Department of Physical and Organic Chemistry

Experimental and computational studies of various physico-chemical processes at surfaces and synthesis of organic and inorganic compounds.

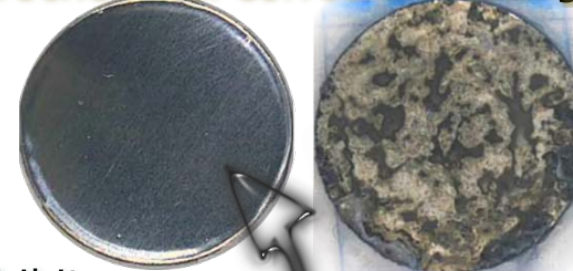
organic synthesis



modeling & simulation

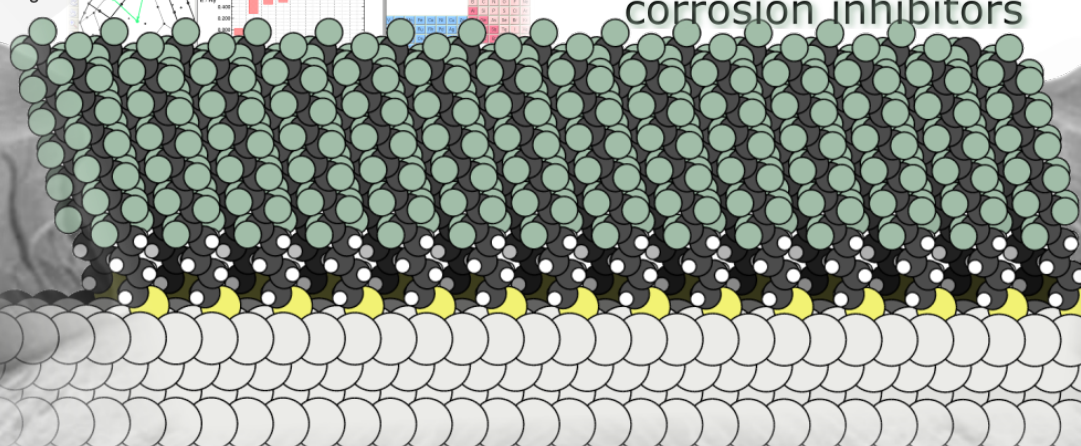
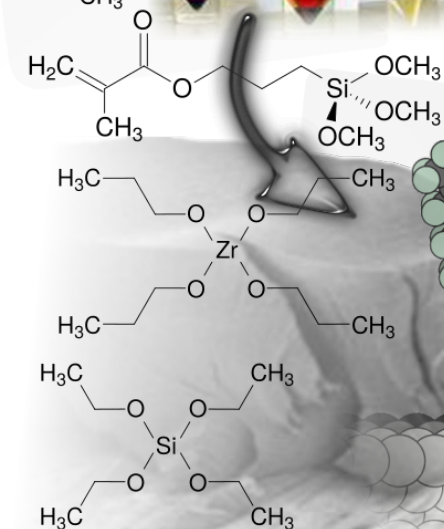


electrochemical corrosion testing



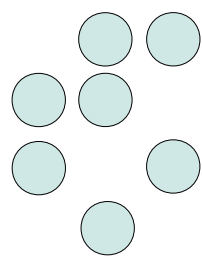
corrosion inhibitors

coating



metal

Program of the QE-2019 Summer School

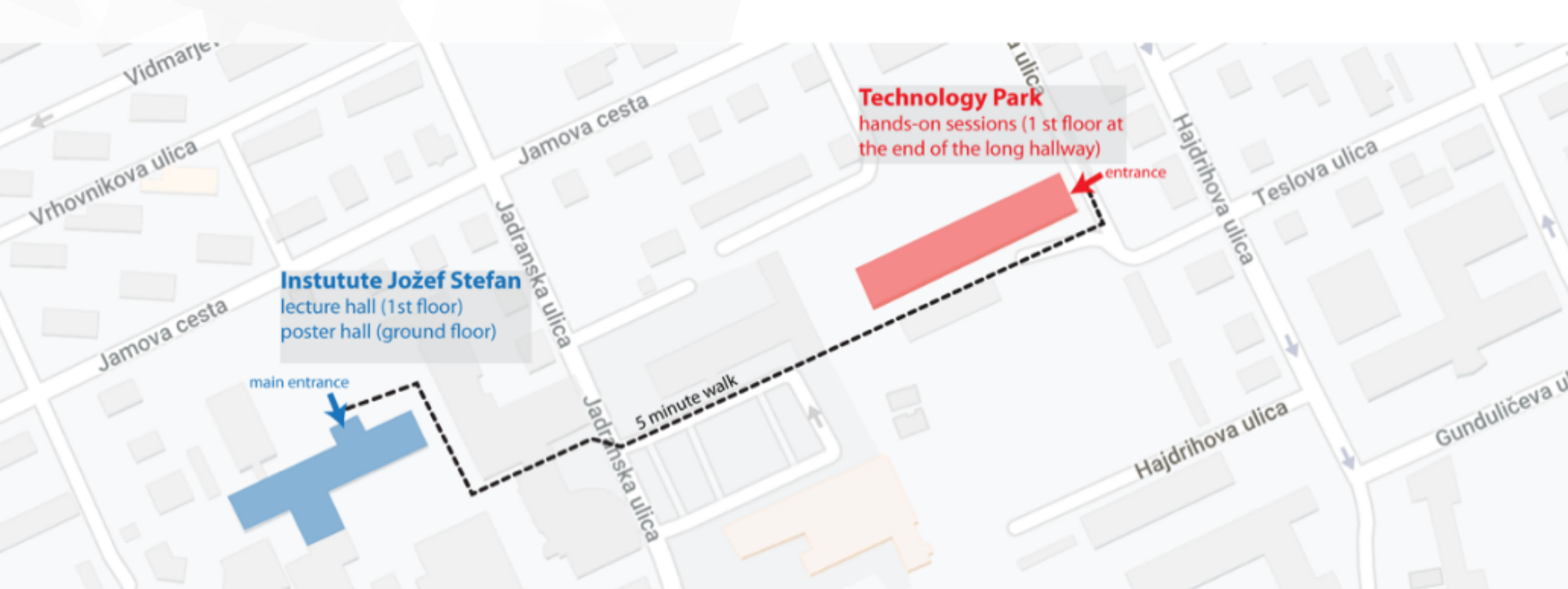
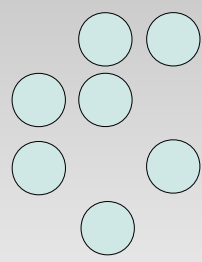


Color code: **Lecture** (lecture-hall) **Hands-on** (classroom)

DAY 1: Monday, September 16

8:00 – 8:50	<i>Registration & participant's computer setup check</i>	
8:50 – 9:00	<i>Opening remarks & general instructions</i>	
9:00 – 10:30	Paolo Giannozzi and Pietro Delugas <i>Quantum ESPRESSO: overview and basic functionalities. The self-consistent cycle. PBC: supercells and k-point sampling.</i>	
10:30 – 11:00	<i>Coffee break</i>	
11:00 – 12:30	Paolo Giannozzi and Pietro Delugas (contd). <i>Charge densities and potentials. Systems in 0-1-2-3D. Metals vs. insulators. Non-magnetic vs. magnetic systems.</i>	
12:30 – 14:00	<i>Lunch</i>	
14:00 – 14:30	<i>Participant's computer setup check (contd).</i>	
14:30 – 18:00	Hands-on. Anton Kokalj, Pietro Delugas, Andrea Urru, Matic Poberžnik, Andrijana Solajić, Jelena Pešić <i>Installation. SCF + basic post-processing. XCrySDen, PWgui, QE-emacs-modes, PWTK (basics). Exercises.</i>	
18:00 – 18:30	<i>Coffee break</i>	
18:30 – 19:30	Special guest lecture – Željko Šljivančanin <i><u>A short introduction to physics and chemistry at crystalline surfaces</u></i>	

Location of the hands-on classroom

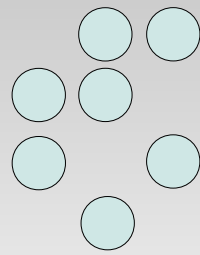


Canteens and restaurants



+ **Hombre** restaurant (near Simbol youth hostel)

Poster sessions



- ▼ **odd # posters on Wed; even # posters on Thu**
(submit elevator pitch slides by **Tue** morning (**odd**) and **Wed** morning (**even**))
- ▼ poster can be mounted on poster-boards tomorrow on Tuesday
(pay attention to poster numbers)

1

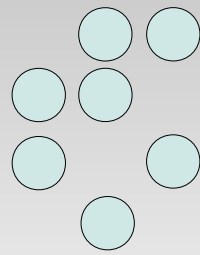
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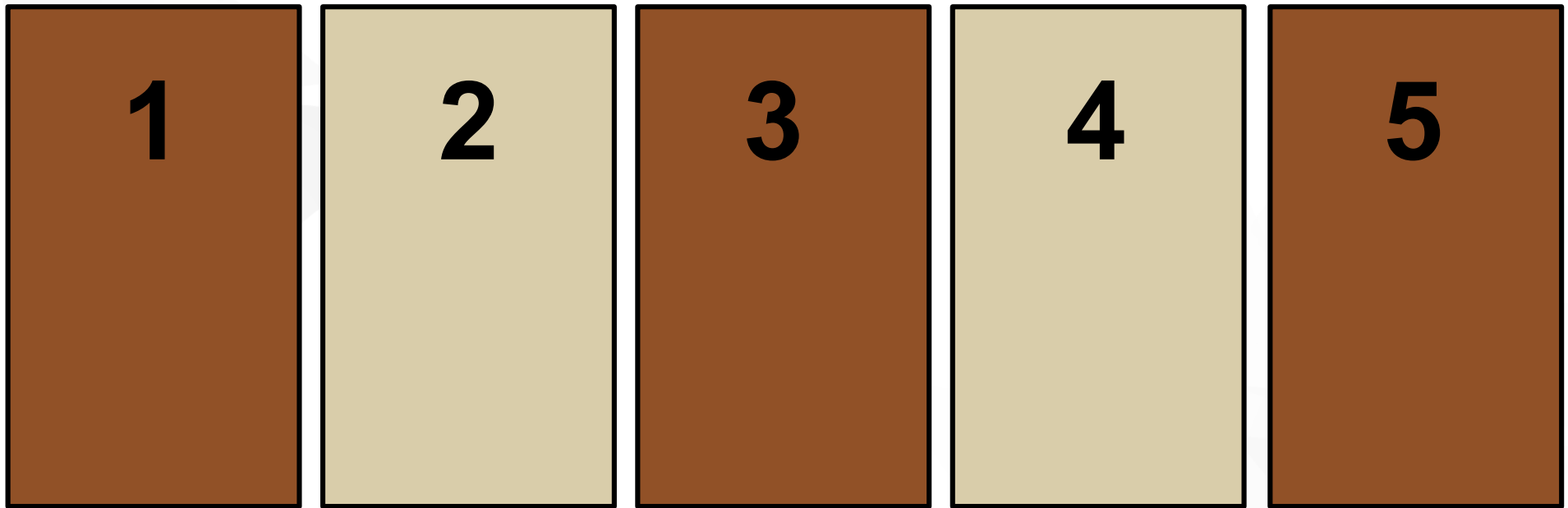
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Poster sessions

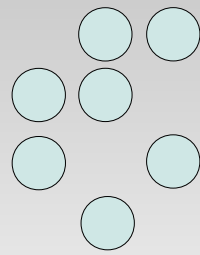


- ▼ **odd # posters on Wed; even # posters on Thu**
(submit elevator pitch slides by **Tue** morning (**odd**) and **Wed** morning (**even**))

Wednesday

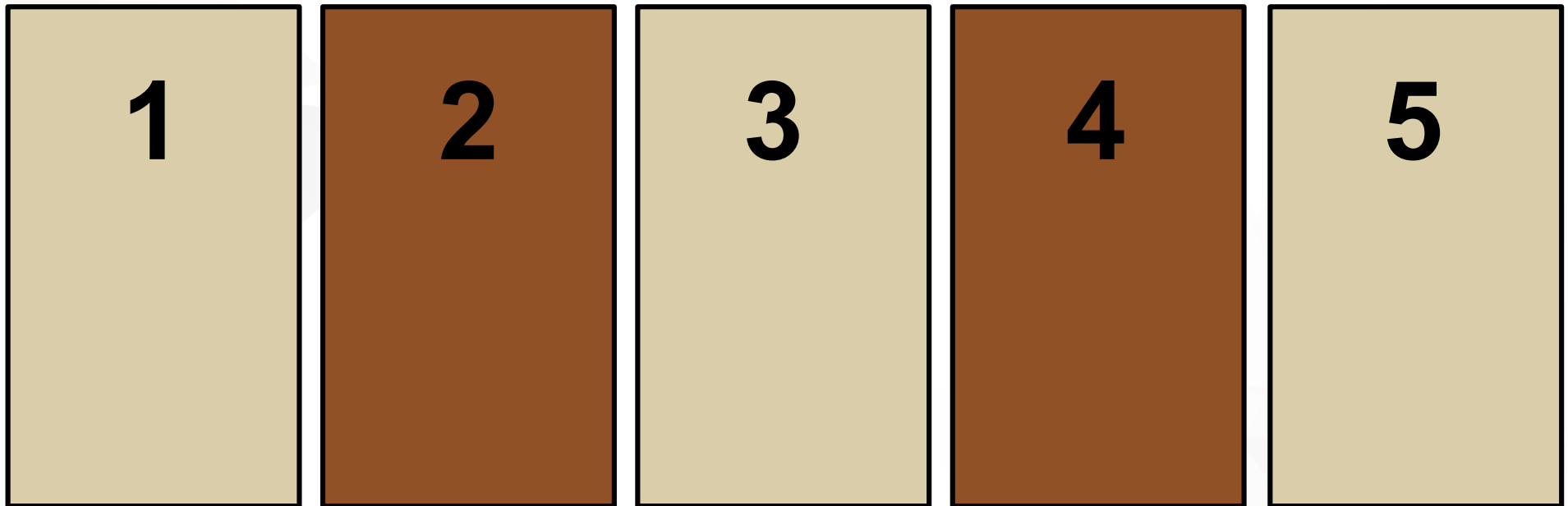


Poster sessions

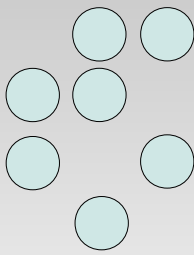


- ▼ **odd # posters on Wed; even # posters on Thu**
(submit elevator pitch slides by **Tue** morning (**odd**) and **Wed** morning (**even**))

Thursday



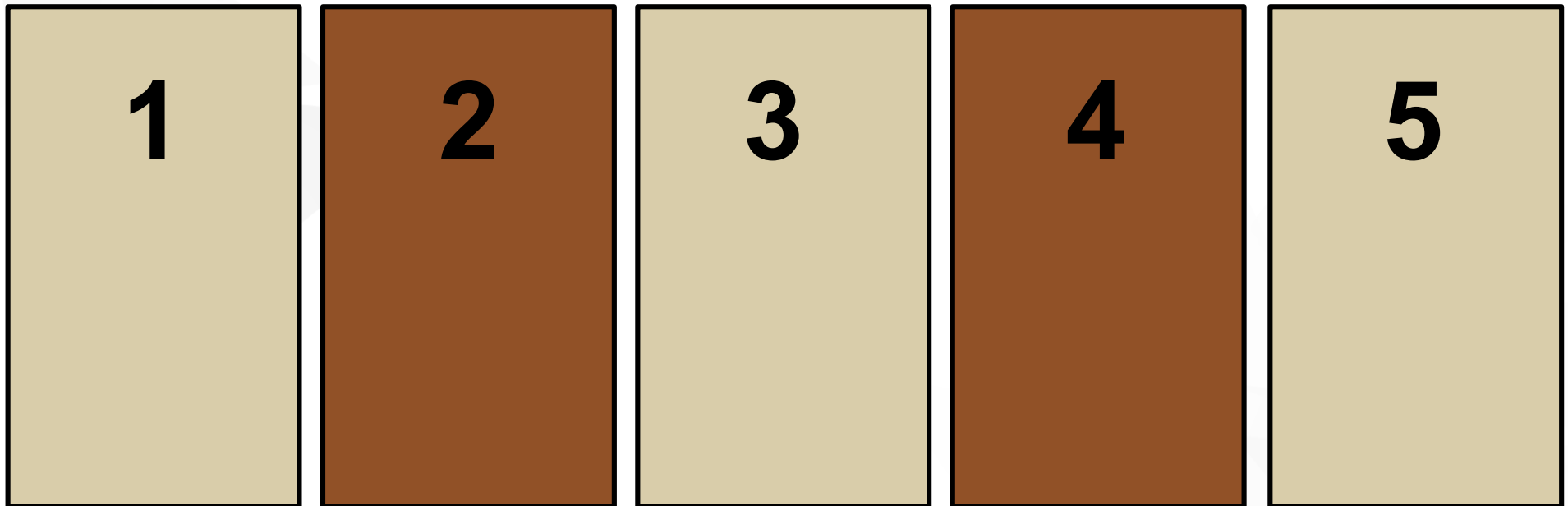
Poster sessions



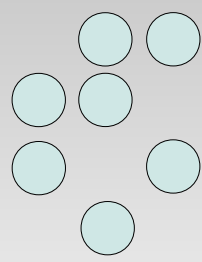
▼ best poster award

(you have a voting ticket – vote by Thursday 21:00)

Thursday



Participant's computer setup check



- ▼ if not yet done: please consult with tutors after lunch

That's all !

