

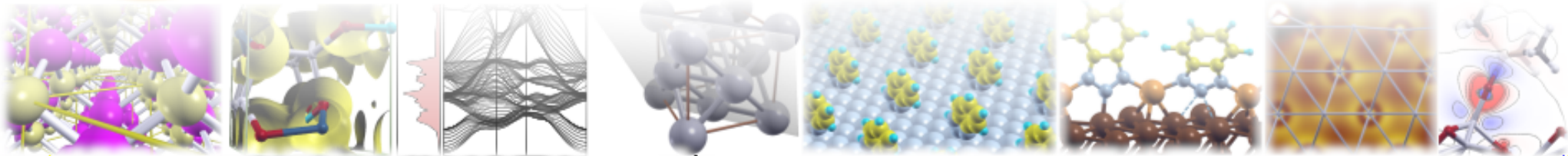


QUANTUMESPRESSO

September 15–20, 2019

Ljubljana, Slovenia

Summer School on Advanced Materials and Molecular Modelling



Closing remarks &

POSTER PRIZE AWARD



QUANTUM ESPRESSO
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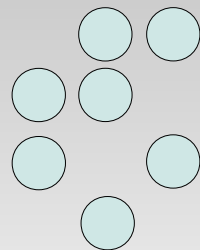
MAX DRIVING
THE EXASCALE
TRANSITION

 Jožef Stefan
Institute
Ljubljana, Slovenija

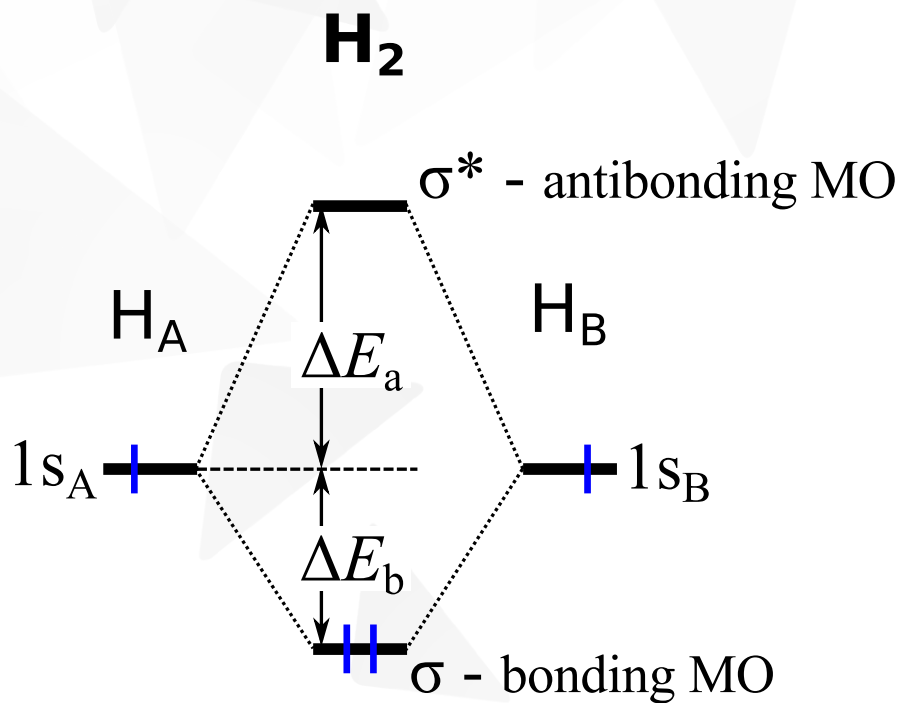
 **cecam**
Centre Européen de Calcul Atomique et Moléculaire

 **EUROTECH**
Imagine. Build. Succeed.

A chemist's view of bonding



▼ molecular orbital (MO) diagram



net attraction

(two-orbital two-electron interaction)

$$\Delta E_a = + \frac{H_{AB}}{1 - S_{AB}}$$

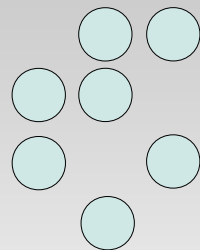
$$\Delta E_b = - \frac{H_{AB}}{1 + S_{AB}}$$

H_{AB} = interaction between s_A & s_B

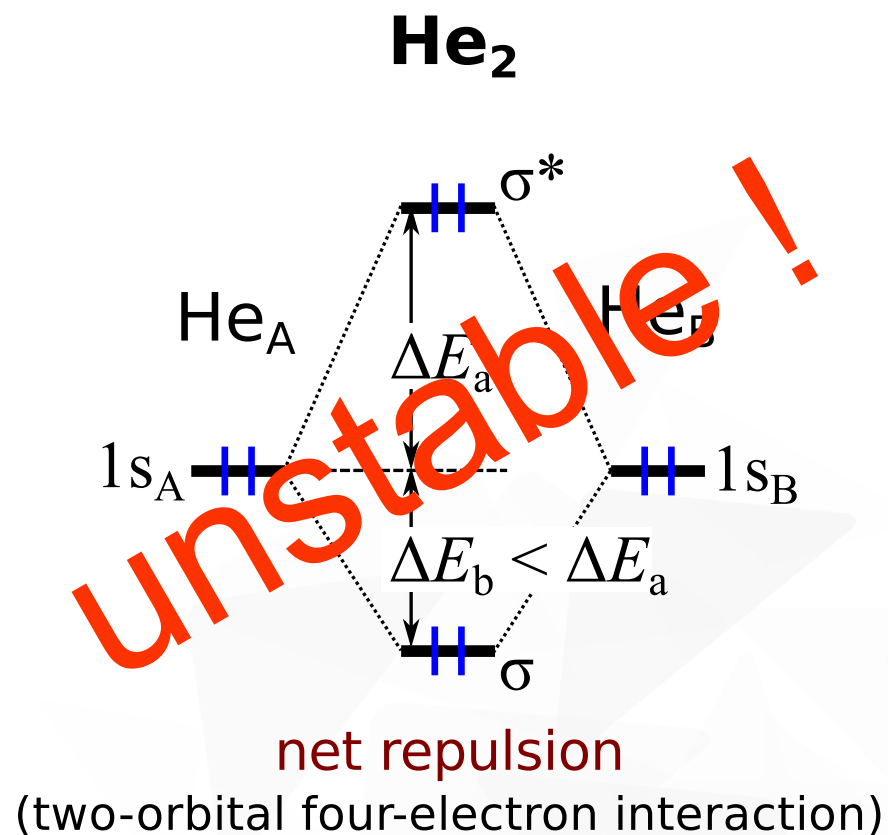
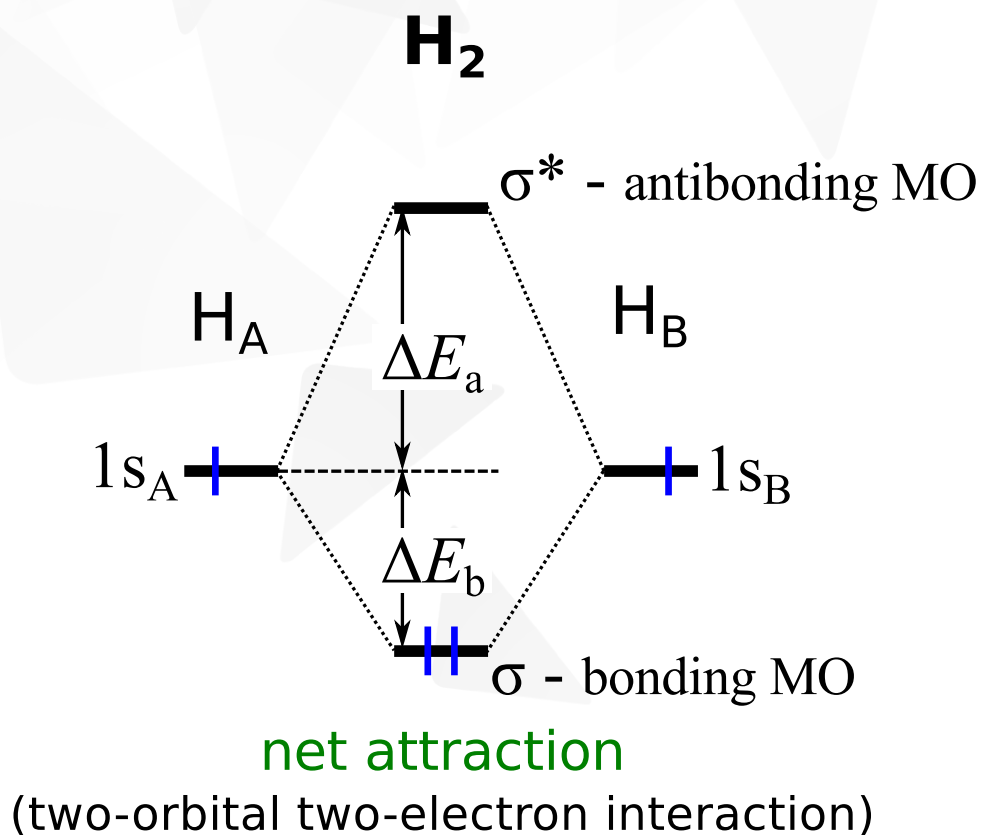
S_{AB} = overlap between s_A & s_B

$$H_{AB} \propto S_{AB}$$

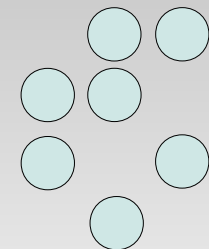
A chemist's view of bonding



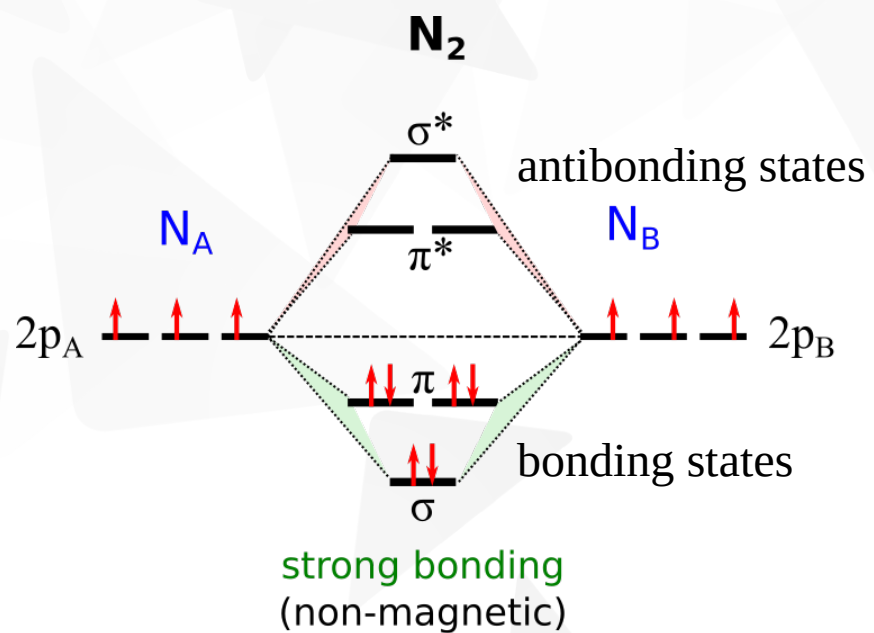
▼ molecular orbital (MO) diagram



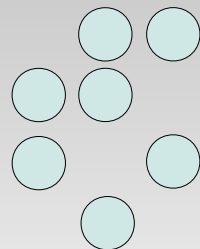
A chemist's view of bonding



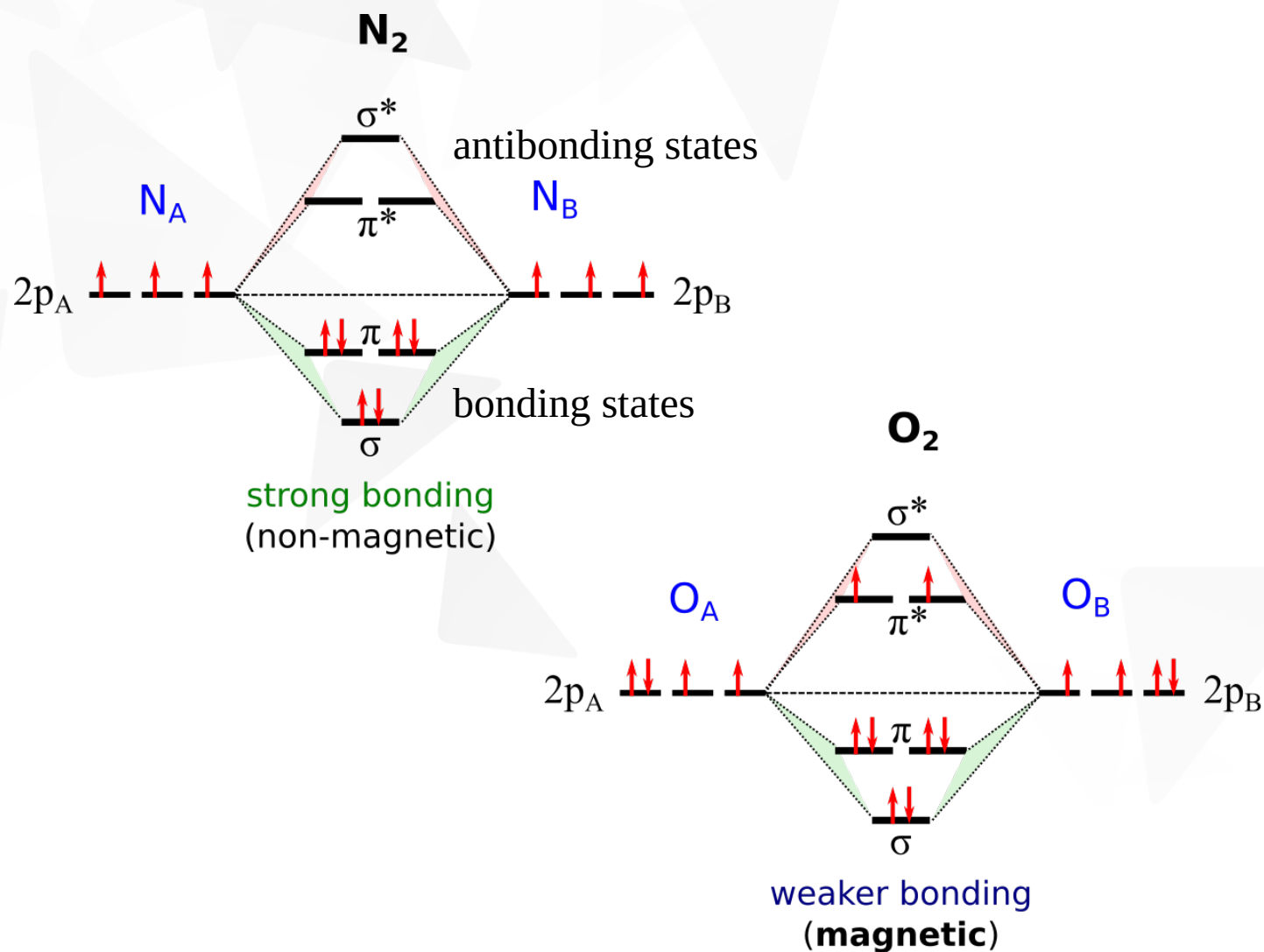
▼ molecular orbital (MO) diagram



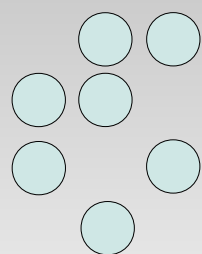
A chemist's view of bonding



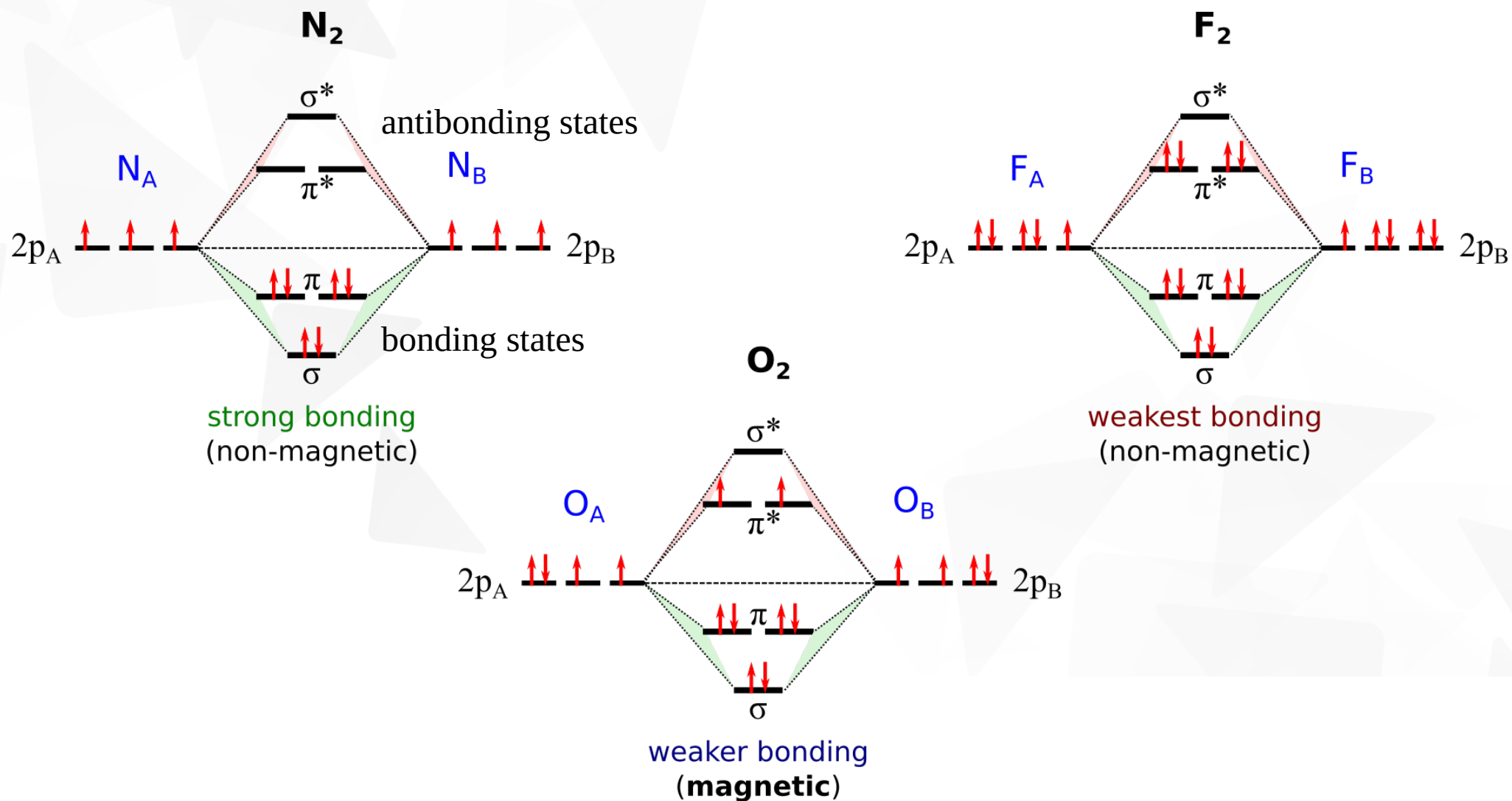
▼ molecular orbital (MO) diagram



A chemist's view of bonding



▼ molecular orbital (MO) diagram

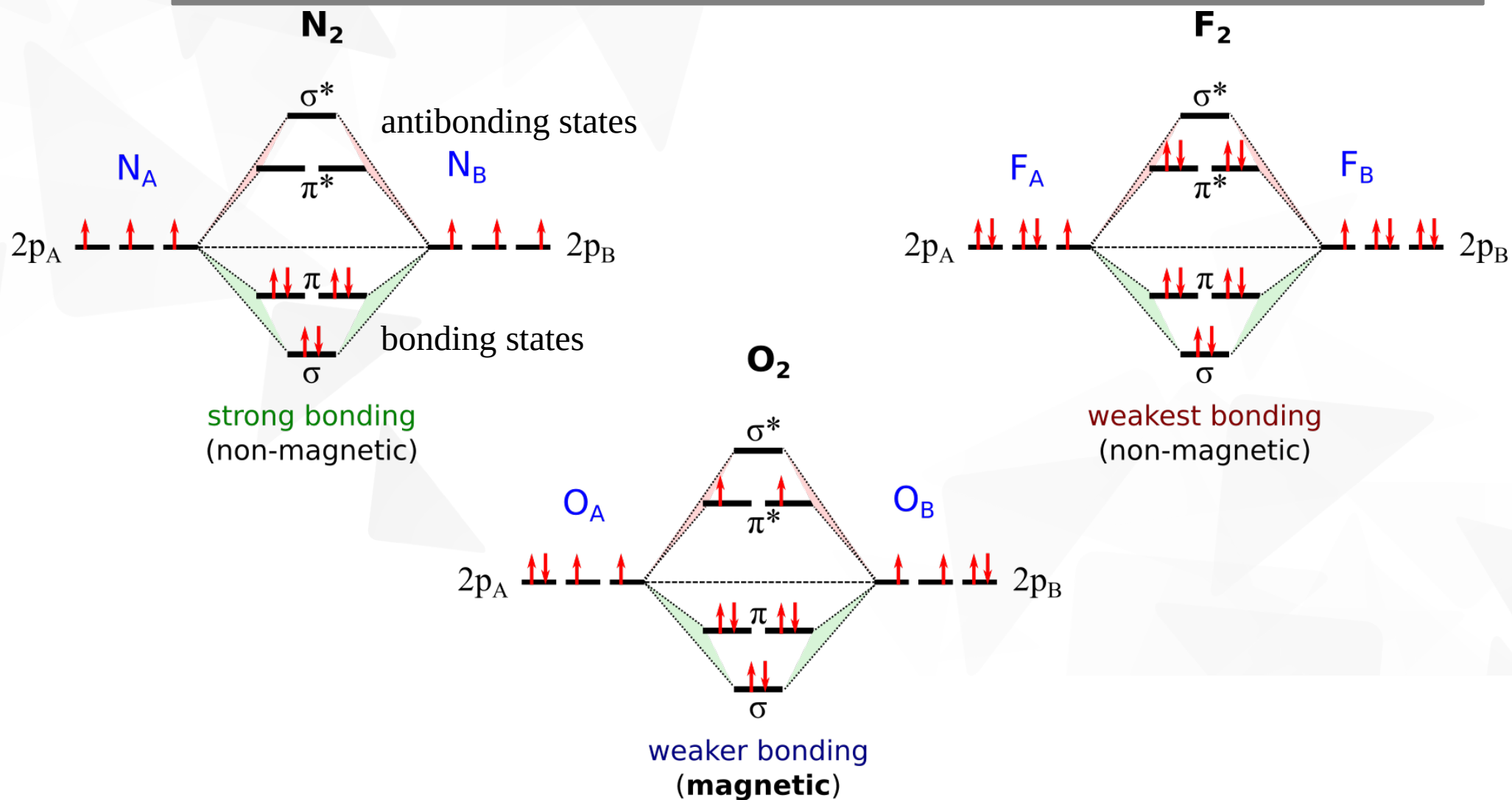


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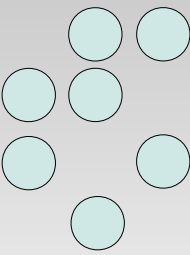
Let's prove it by experiment !

(the movie of the experiment can be seen at http://qe2019.ijs.si/O2_experiment.avi)

▼ mole

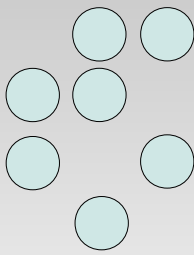


Feedback survey on QE-2019

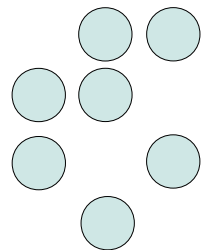


- ▼ We want to hear your feedback so we can keep improving our logistics and content
- ▼ You will receive by email a link to a short on-line survey

Slides of lectures and hands-on sessions



- ▼ Slides of lectures will be available on QE-2019 web-page:
<http://qe2019.ijs.si/>
- ▼ Pictures taken by photographer will be also available there
- ▼ Hands-on are available on gitlab:
<https://gitlab.com/QEF/material-for-ljubljana-qe-summer-school>



Poster price award

- ▼ 46 voted
(45 valid and 1 invalid ballot ticket)
- ▼ organizing committee selected 5 posters without ranking them
(rule: the poster who receives the most votes among these 5 is a winner)

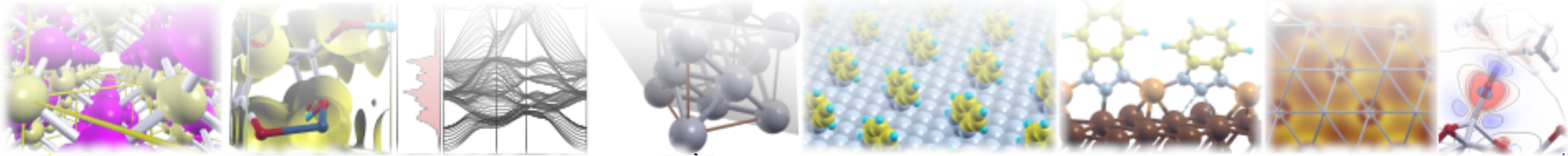


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POSTER PRIZE AWARD

GOES TO



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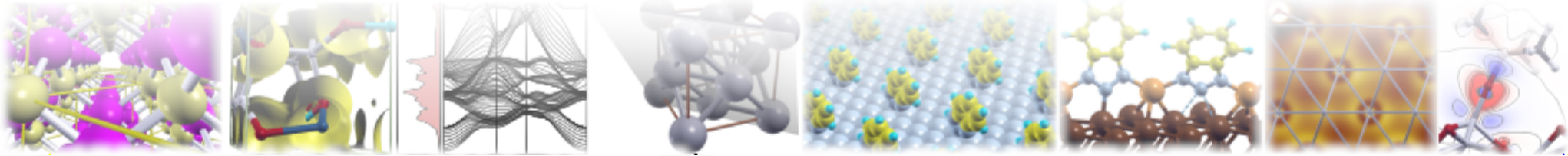


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POSTER #.22: Matic Poberžnik

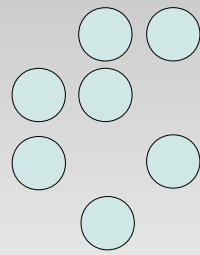
Lateral interactions between electronegative adatoms on metal surfaces: a high-throughput computational study

CONGRATULATIONS !



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Poster price award ballot results



▼ voting results for the 5 posters selected by the committee:

1) Matic Poberžnik – 9 votes

2) Marion Antonia van Midden – 6 votes

3) Matjaž Dlouhy – 4 votes

4-5) Matteo Busato – 2 votes

4-5) Srdjan Stavrić – 2 votes

▼ ranking according to voting of participants:

1) Matic Poberžnik (#22) – 9 votes

2) Marion Antonia van Midden (#7) – 6 votes

3) Marie Kempkes (#24) – 5 votes

4) Matjaž Dlouhy (#27) – 4 votes

5) Chiara Ribaldone (#5) – 3 votes

poster ID

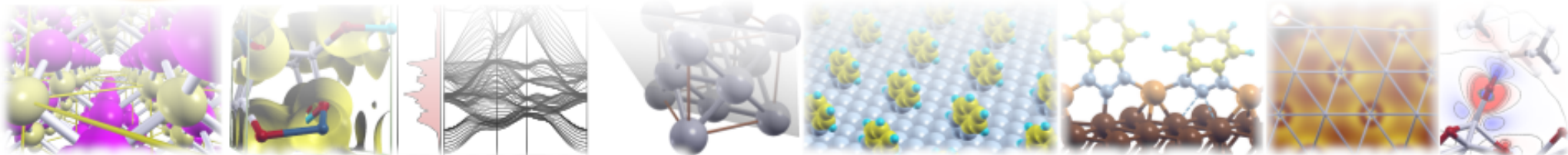


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THANK YOU FOR COMMMING

FAREWELL



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