

PWF Tunisia: Computational Materials Science based on Density-Functional Theory for Renewable Energy and Spintronics

From 16th to 27th September 2024



The Abdus Salam
**International Centre
for Theoretical Physics**
Physics Without Frontiers



The background image shows a university gate with a sign that reads "FACULTE DES SCIENCES DE TUNIS" in French and Arabic. The gate is flanked by trees and a fence. The text "Current Situation for Computational Physics" is overlaid on the image in a large, bold, black font.

Current Situation for Computational Physics



- In the Faculty of Sciences of Tunis, there is a notable absence of computational materials science.



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- Important issue as the FST belongs to the highest-ranking University in *Tunisia* and one of the scientific centers of the *region*.
- The situation is similar in the other scientific departments across the country.
- A big loss for the country as computational materials science offers many possibilities for university-industry partnership and does not require significant financial starting investment.

The background image shows the entrance gate of the Faculty of Sciences of Tunis. The gate is a dark metal structure with a sign on top. The sign features a logo on the left and text in Arabic and French. The Arabic text reads 'كلية العلوم بتونس' and the French text reads 'FACULTE DES SCIENCES DE TUNIS'. A red flag is flying on a pole to the right of the gate. The scene is set against a backdrop of trees and a clear sky.

كلية العلوم بتونس
FACULTE DES SCIENCES DE TUNIS



Goals of Our Project



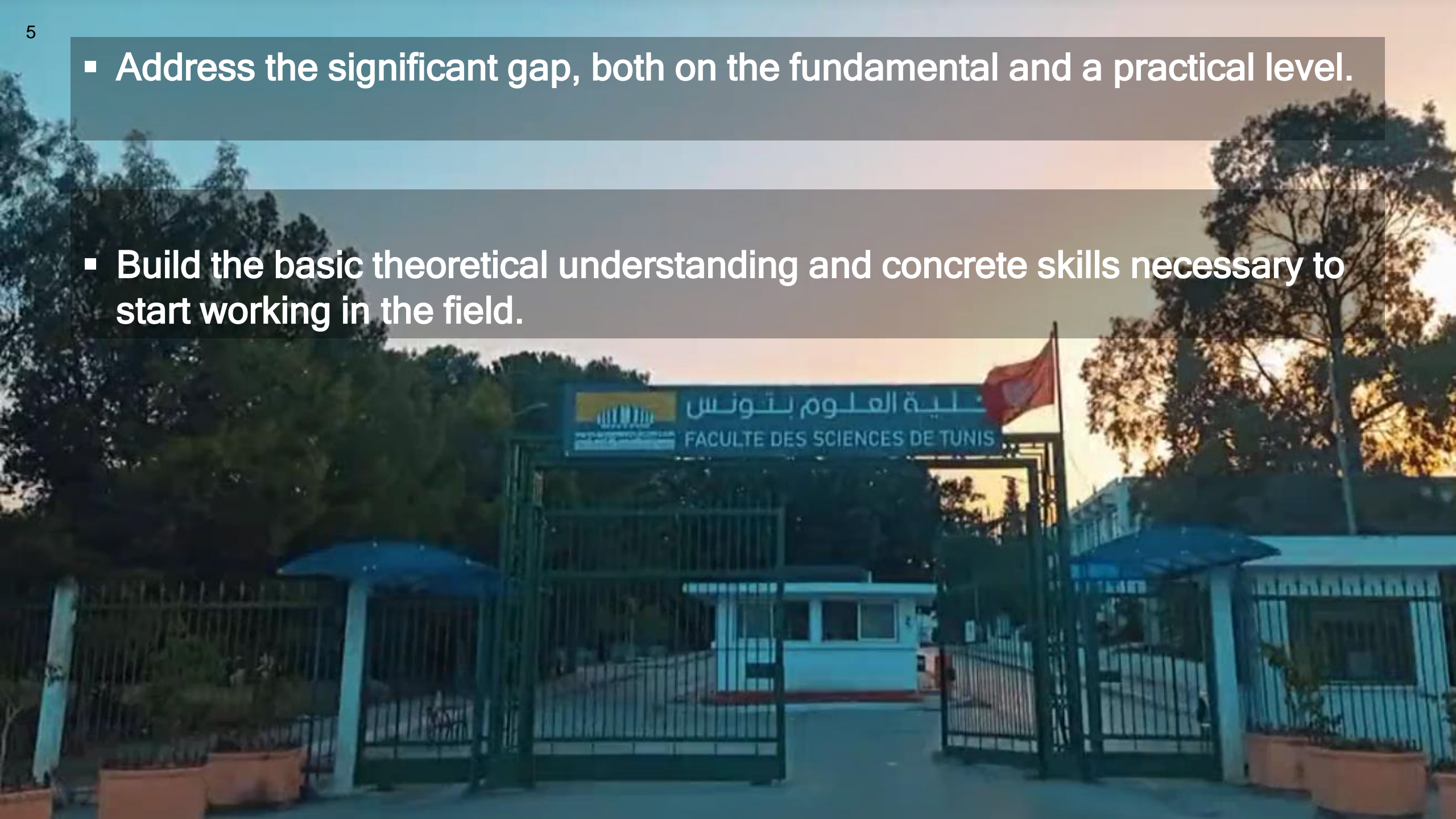
كلية العلوم بتونس
FACULTE DES SCIENCES DE TUNIS



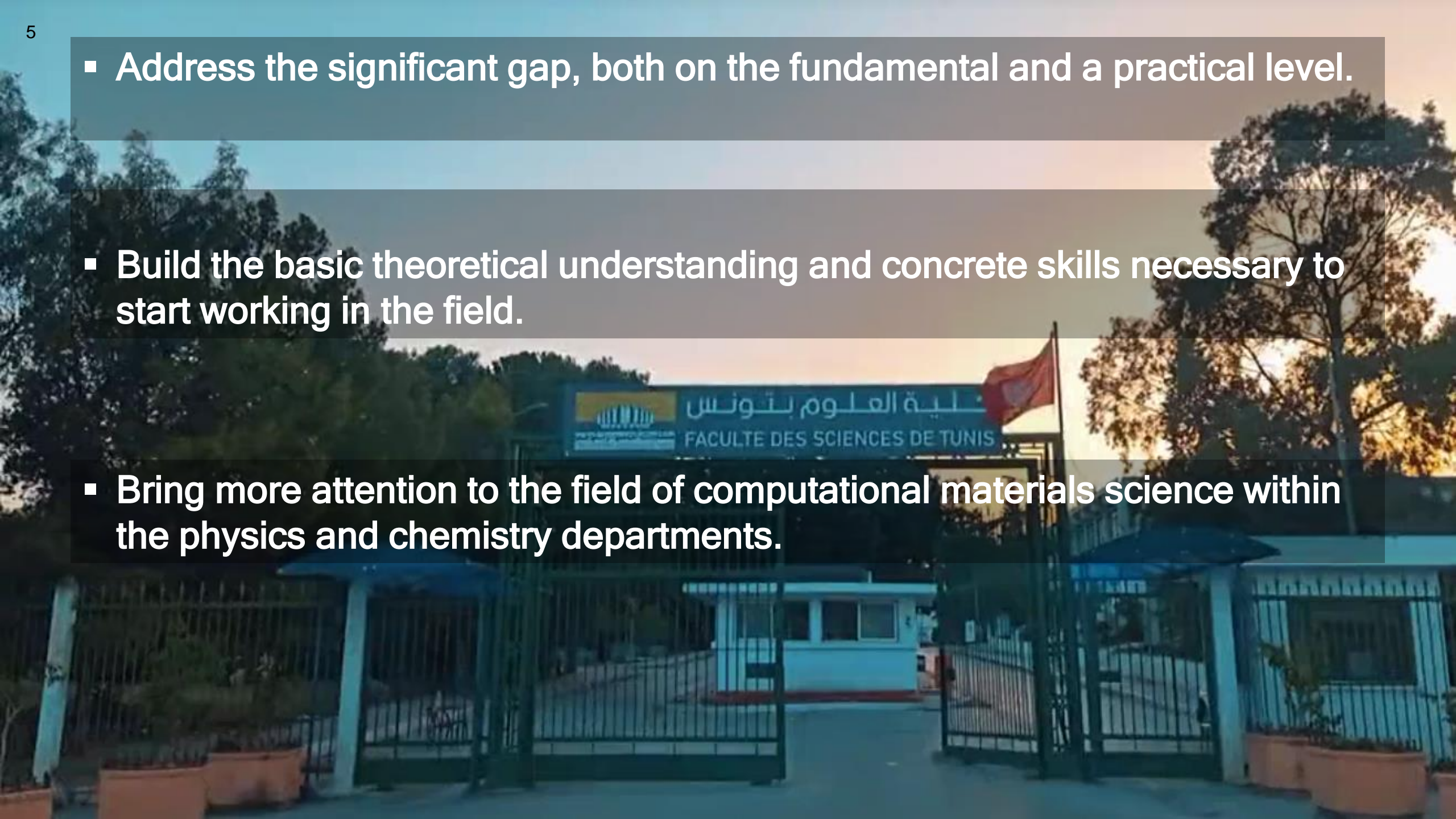
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- Foster students' familiarity and interest in the area.

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كلية العلوم بتونس
FACULTE DES SCIENCES DE TUNIS

- Address the significant gap, both on the fundamental and a practical level.
- Build the basic theoretical understanding and concrete skills necessary to start working in the field.
- Bring more attention to the field of computational materials science within the physics and chemistry departments.
- Foster students' familiarity and interest in the area.
- Establish new branch of research and collaborations focused on the topics covered in the project.



الكلية العلوم بتونس
FACULTE DES SCIENCES DE TUNIS



Our Team



Maha Hsouna
SISSA-ICTP



Nataša Stojić
ICTP



Anita Yadav
ICTP



Nicola Seriani
ICTP



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Walid Ouerghi
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Khoulood Chika
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Ghassen Jemai
FST



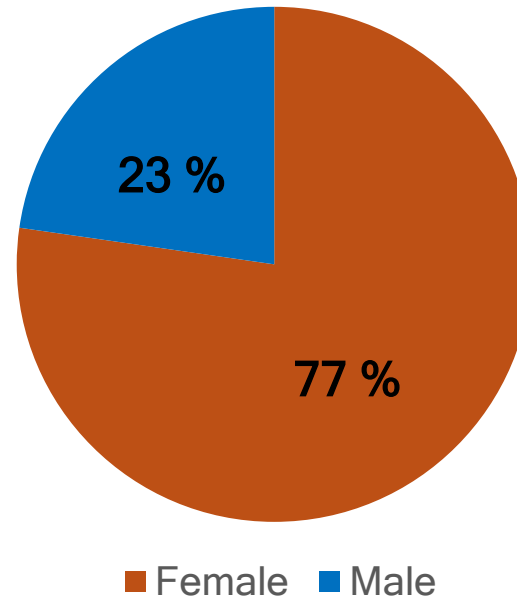
Mehdi Arfaoui
FST



Participants

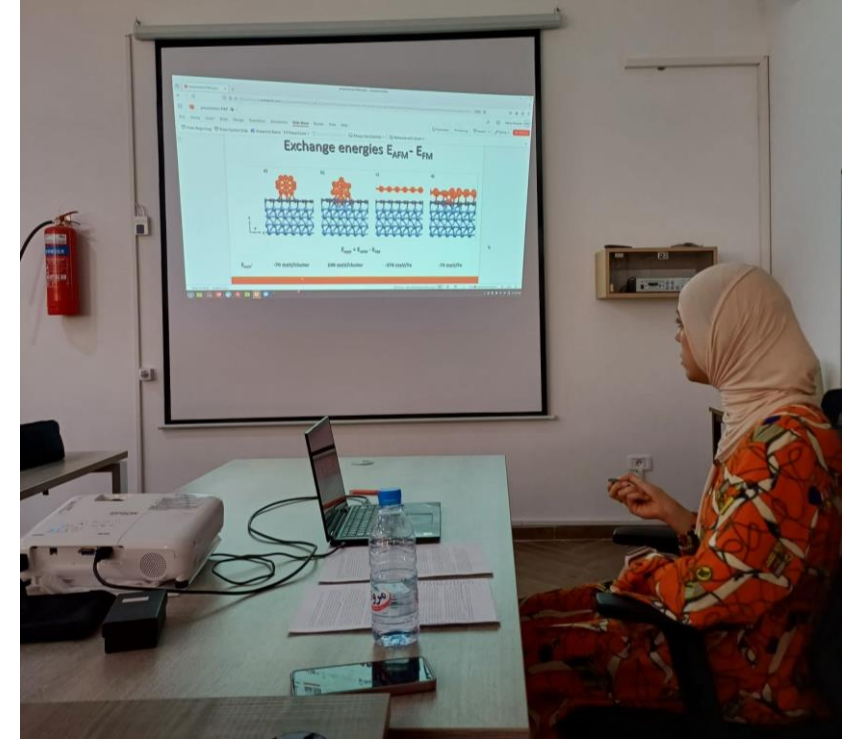


The 22 participants were from various scientific institutes in Tunisia!





Highlights of the Activities



The morning sessions were dedicated to:

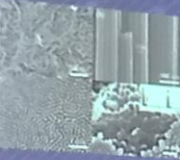
- Lectures on basic solid-state theory
- Introduction to density-functional theory
- Introduction to spintronics and renewable energy




Zoom Meeting
This meeting needs security. Lock Meeting

Nanostructured functional materials


- Materials operate in a complex environment that affects their composition, surface termination, electronic properties, nanomorphology,...
- This has consequences for their functionality



TiO₂ nanotubes as anode material for dye-sensitized solar cells
Li et al., Chem. Mater. 22, 5707 (2010)



Platinum nanoparticles for fuel cells
Kimanicky et al., Electrochim. Acta 55, 7934 (2010)



Silicon nanowires as anode for Li batteries
Chen et al., Adv. Funct. Mater. 20, 4364 (2010)

Zoom Meeting interface with participant thumbnails: Anita Yadav, Zribi, Nisha Mammen.

Making A Better Catalyst -3

- Change the shape of the catalyst particle.

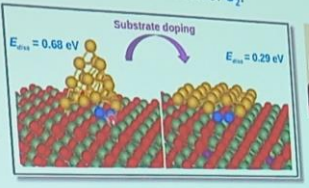
Consider E_{diss} barrier for dissociation of O₂:

O₂

Au

Al


MgO



Substrate doping

$E_{diss} = 0.68 \text{ eV}$

$E_{diss} = 0.29 \text{ eV}$



Nisha Mammen

Mammen, Narasimhan, & Grunwald, J. Am. Chem. Soc., 131, 2003 (2009)
Mammen, de Grunwald and Narasimhan, J. Chem. Phys., 121, 10407 (2004)

Shobhana Narasimhan, INCASR



Wannier90 code

$(A_{\mathbf{k}})_{mn} = \langle \psi_{m\mathbf{k}} | g_n \rangle$

Wannier code

$U(\mathbf{k})$

Ab-initio code

$M_{mn}^{(\mathbf{k},\mathbf{b})} = \langle u_{m\mathbf{k}} | u_{n,\mathbf{k}+\mathbf{b}} \rangle$

WF defined in basis of Bloch states

Modular design in F95
standalone program
library routines available

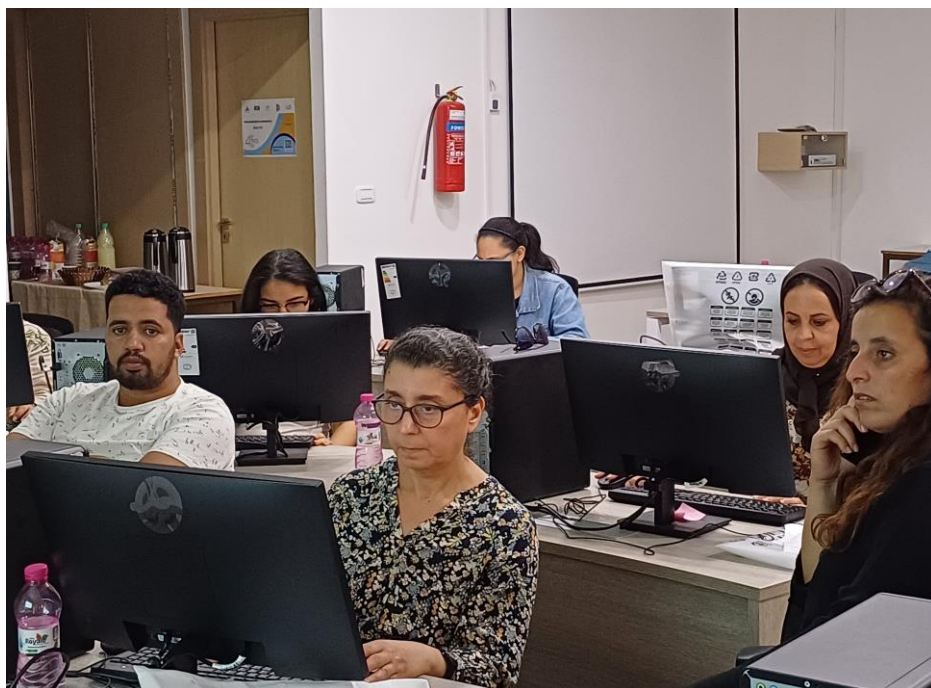
Independent of basis set / methodology used in ab-initio code

24/09/24

Vitalie - PWY TUNISIA 2024



Online lectures on specific topics were given by experts in the field



Long hands-on sessions were dedicated to first introducing DFT using Quantum Espresso and then applying it to more advanced examples

- The students learned about opportunities at ICTP.
- They are already looking to apply to schools and other programmes at ICTP and elsewhere.
- The connections between ICTP and FST have been made which will continue in the future.

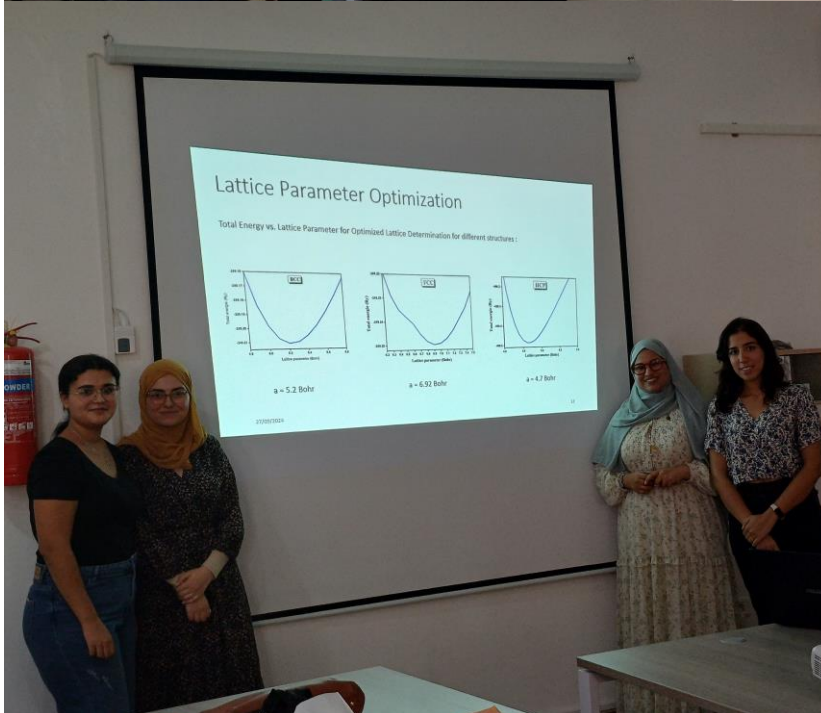




Evaluation & Students Presentations



Small projects were given to the students in which they worked in groups, and they presented their results





Students Feedback



Aycha

This experience not only enhanced my computational skills but also enabled inspiring exchanges with participants from diverse backgrounds, all united by a shared passion for materials science and sustainable applications. I am grateful to ICTP and the trainers for their high-quality guidance and for organizing such a valuable program that will undoubtedly contribute to my academic and



Nour Elhouda

This school deepened my understanding of computational material science. The hands-on approach made the learning experience both practical and engaging, and I feel much more confident in applying these methods. It was inspiring to exchange ideas, share knowledge, and work alongside such a diverse group of talented individuals. These connections made the experience even more special.



Chaima

I had the privilege to attend the PWF School. It was my first experience with such a training program, and it turned out to be incredibly rewarding. **I am deeply grateful to the trainers and organizers for their excellent work, as the program was exceptionally well-structured and informative.** I gained a wealth of knowledge and new skills, and I look forward to applying them in my future research.



Future Directions



- Help find available high-performance computing resources
- Foster international collaborations in the field of computational materials science, particularly with the neighboring Maghreb countries
- Expand scientific exchanges between FST and ICTP at all levels and help organise more activities locally