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

IAEA International Atomic Energy Agency

unesco United Nations Educational, Scientific and Cultural Organization

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FACULTE DES SCIENCES DE TUNIS

Current Situation for Computational Physics


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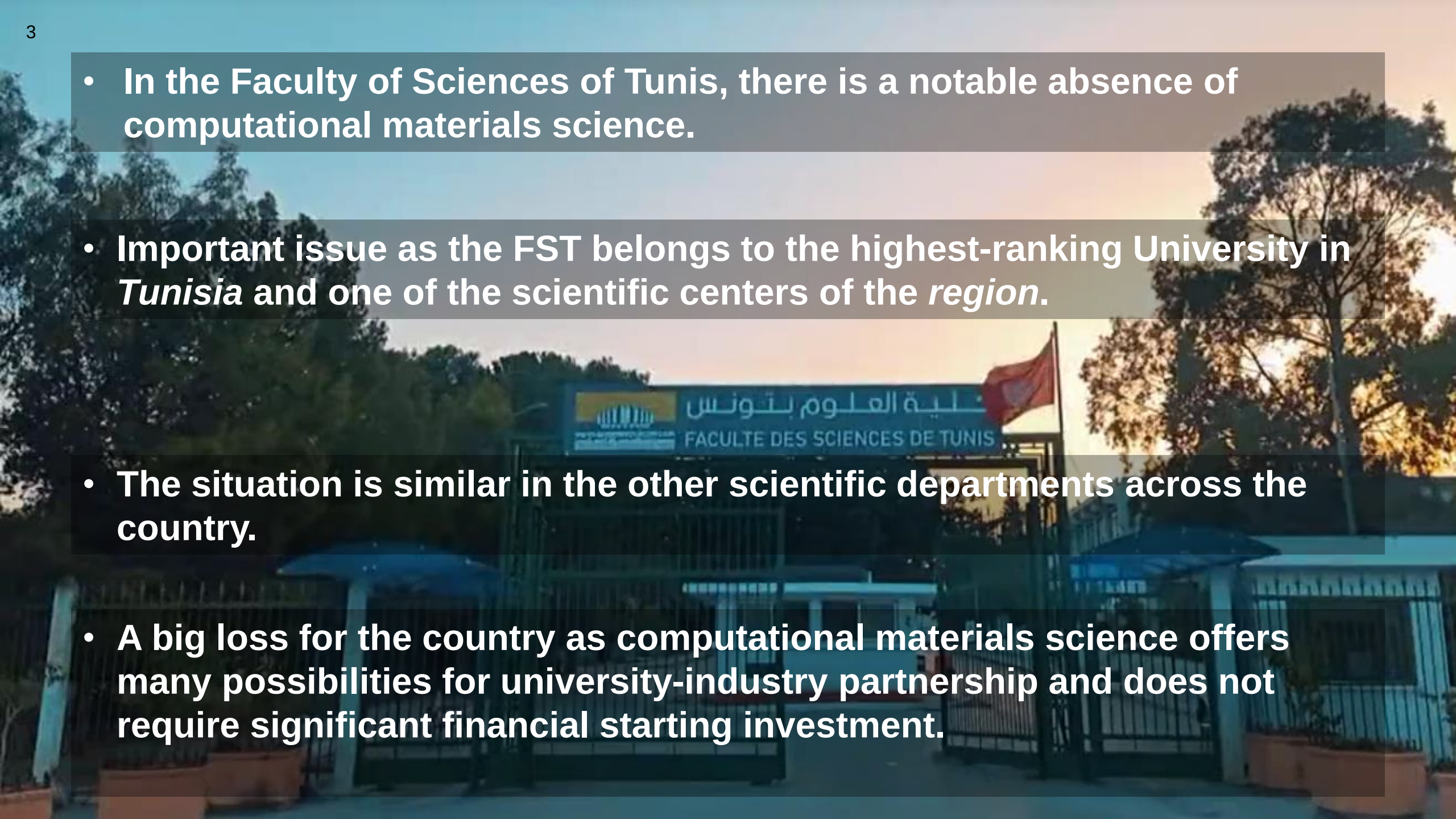

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- **Important issue as the FST belongs to the highest-ranking University in *Tunisia* and one of the scientific centers of the *region*.**
- **The situation is similar in the other scientific departments across the country.**
- **A big loss for the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

Goals of Our Project


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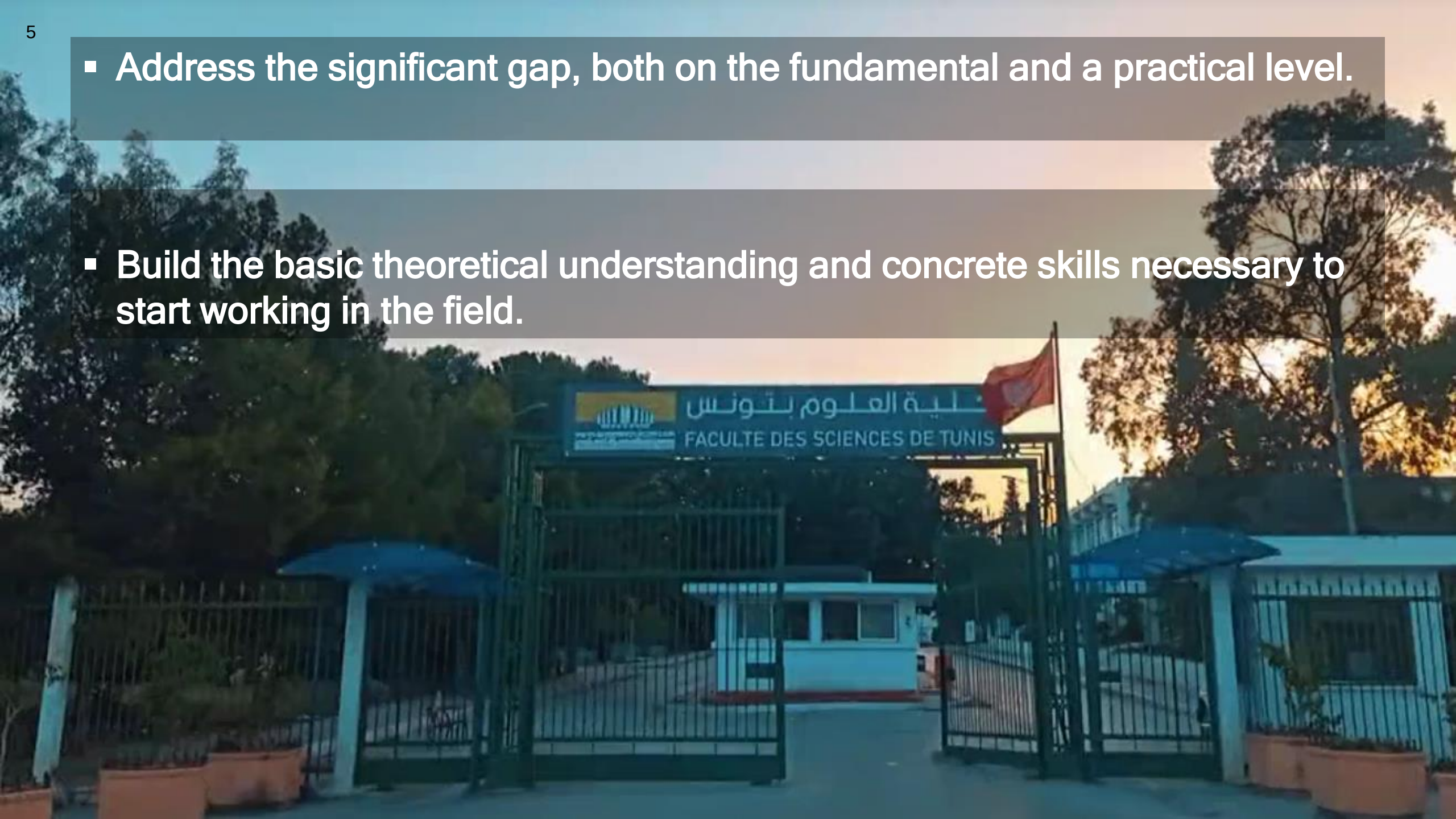
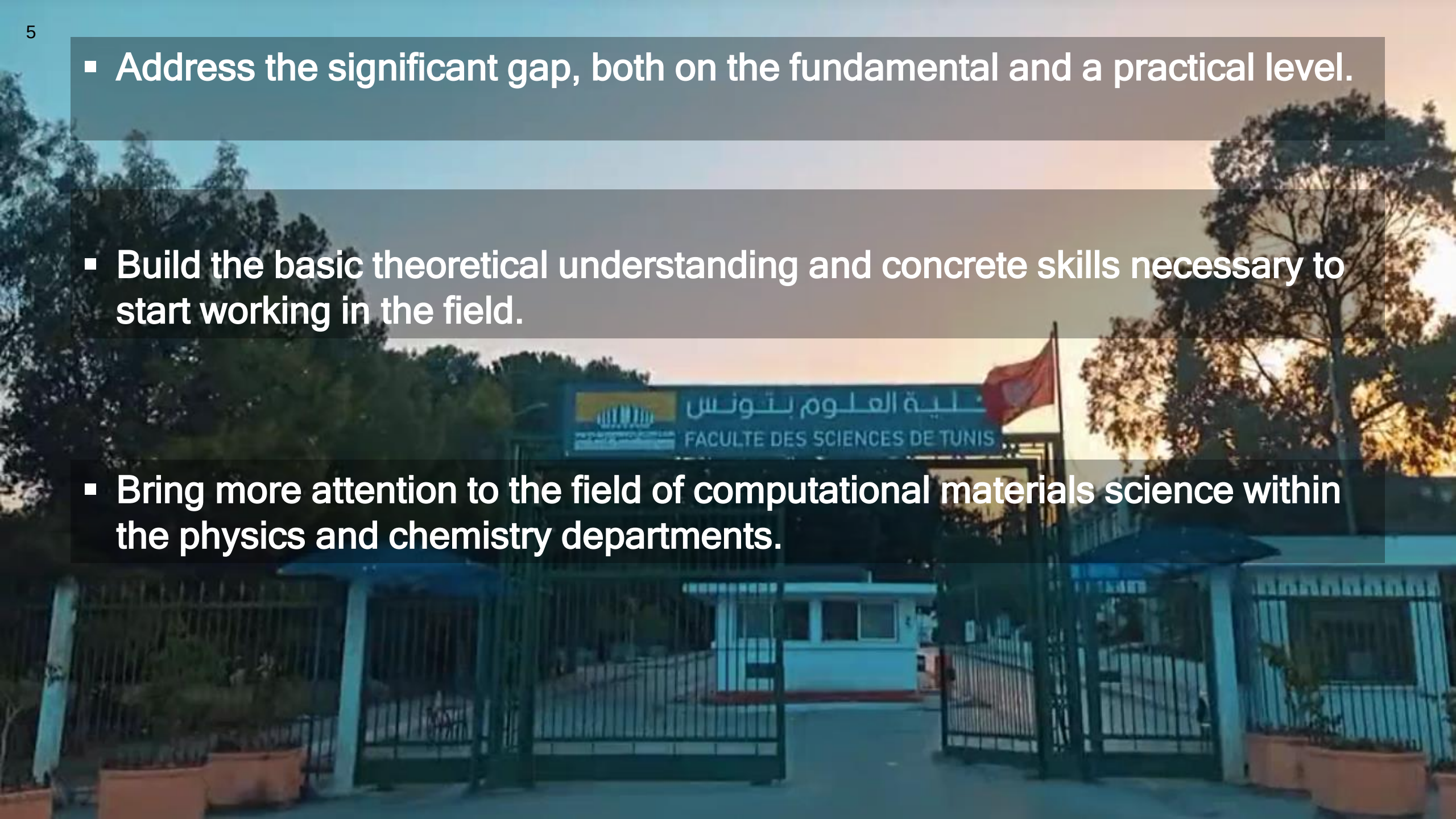
- Build the basic theoretical understanding and concrete skills necessary to start working in the field.





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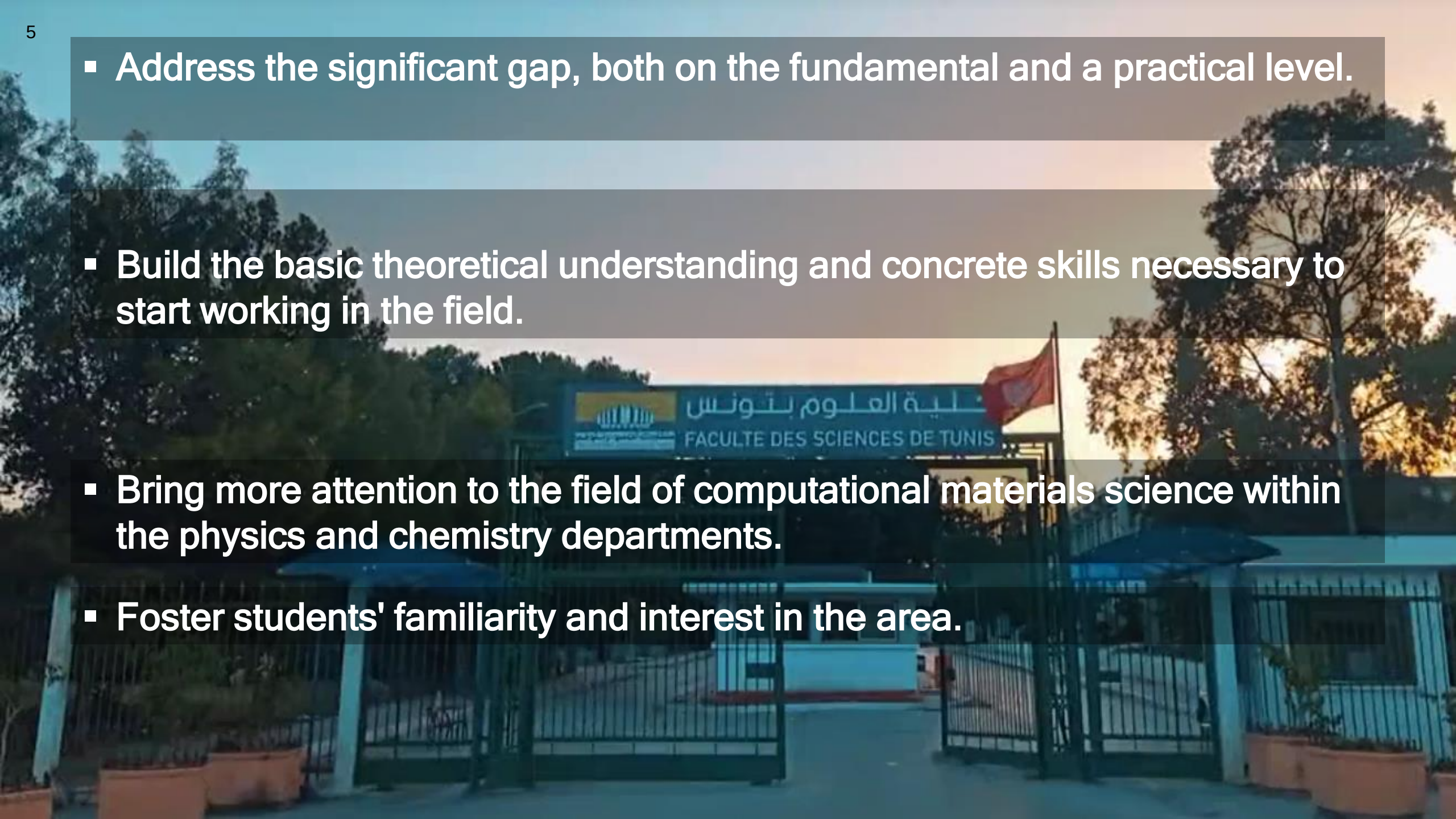
- Bring more attention to the field of computational materials science within the physics and chemistry departments.



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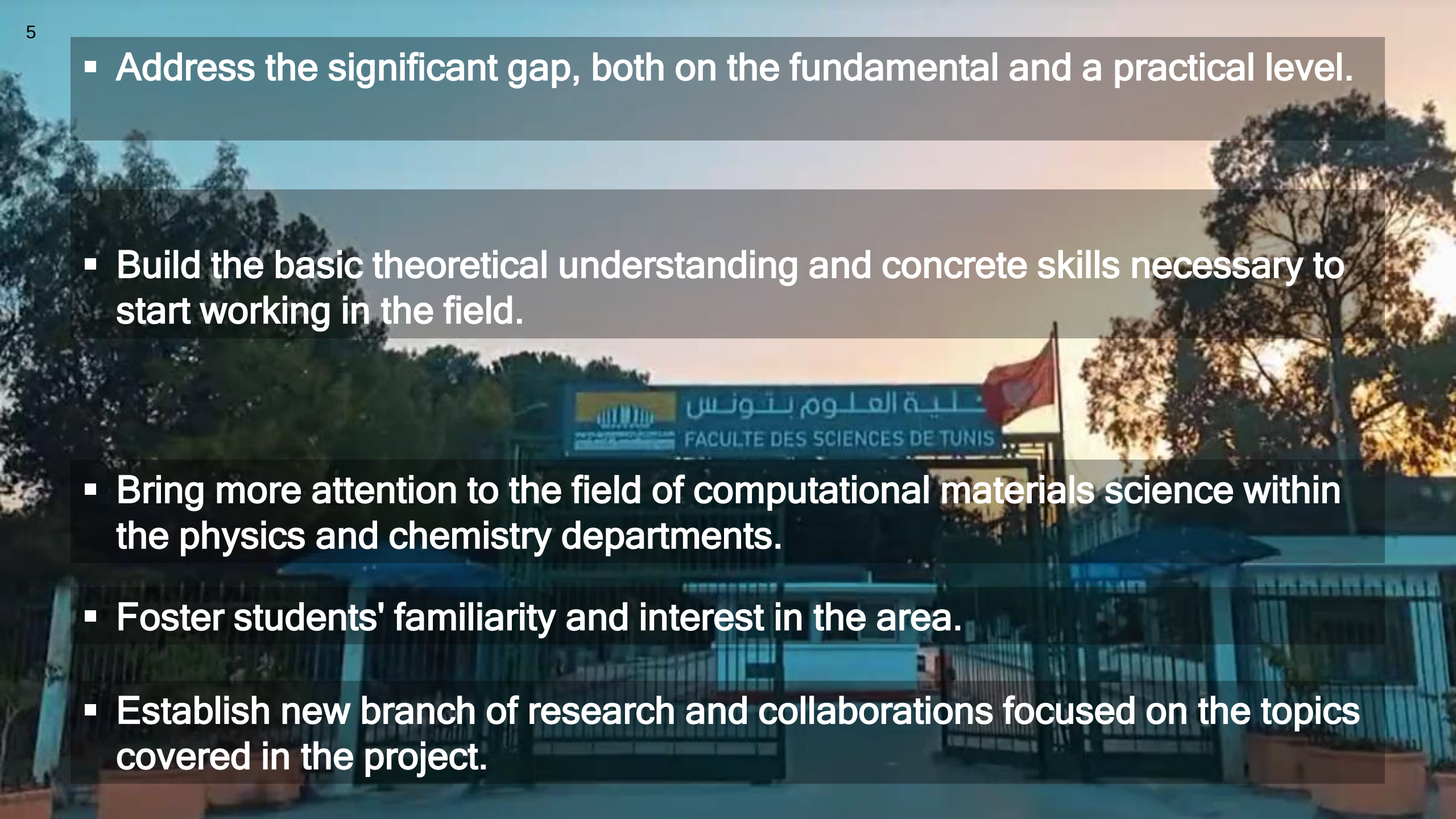

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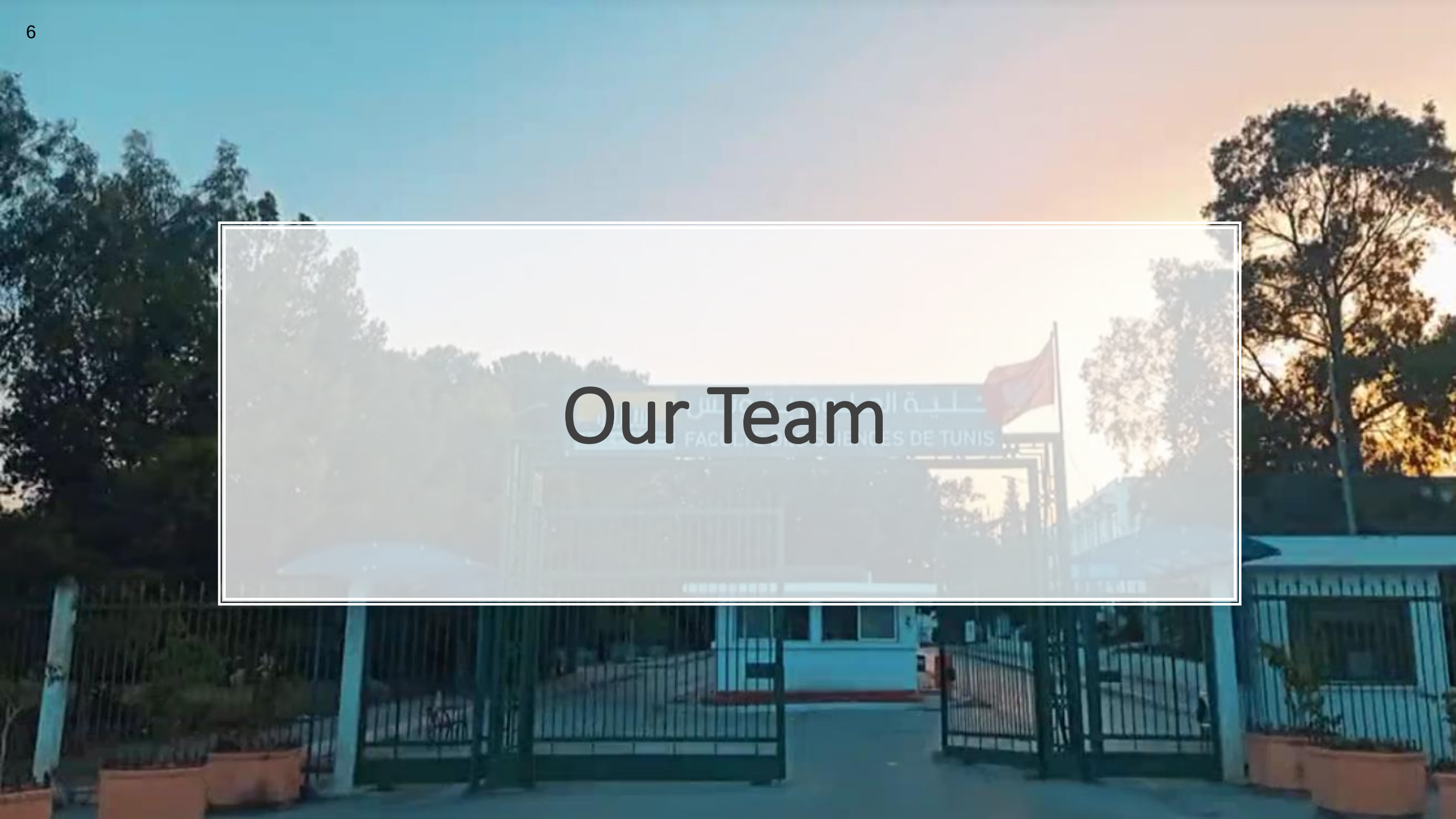
- Establish new branch of research and collaborations focused on the topics covered in the project.



Our Team

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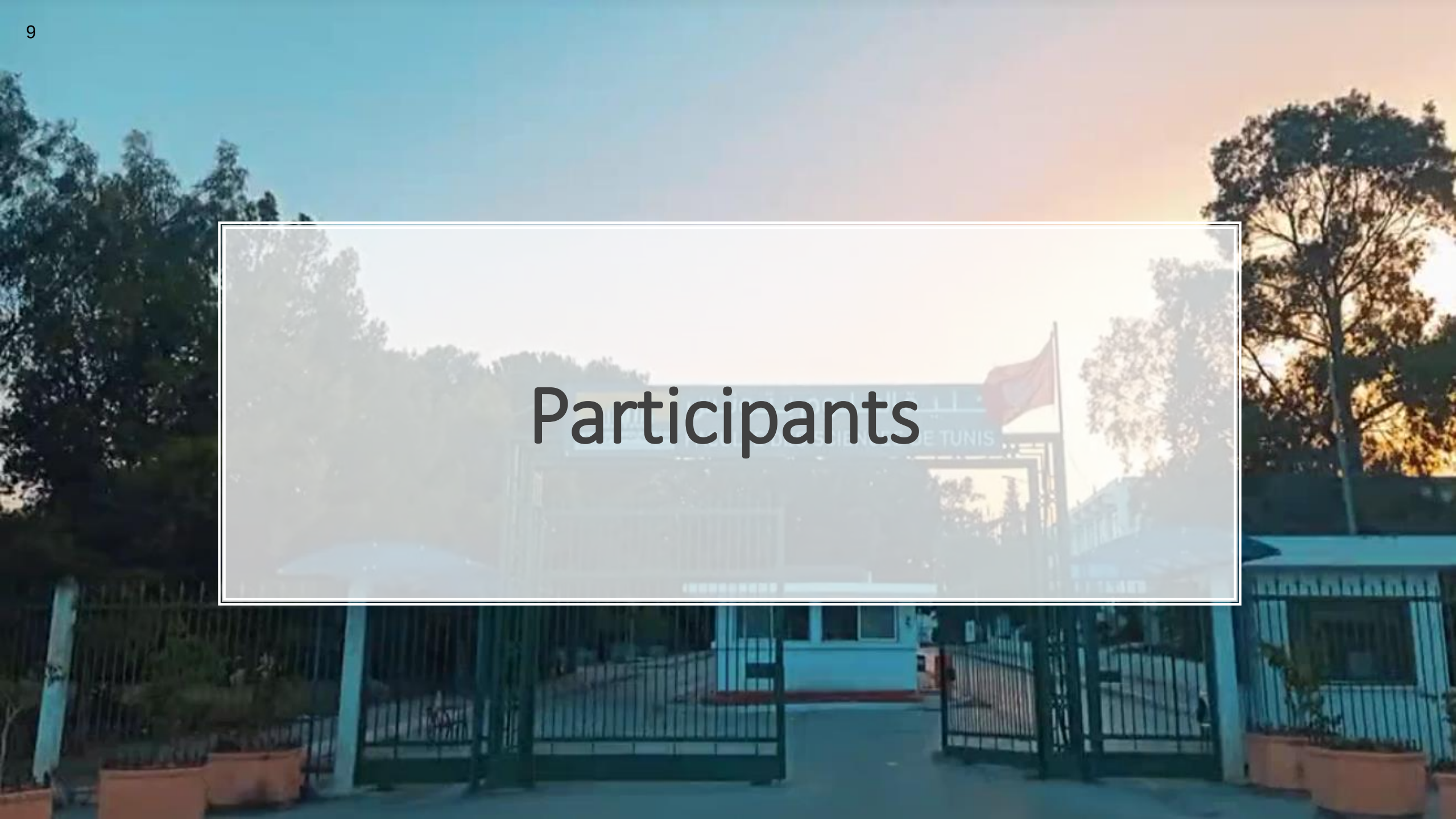
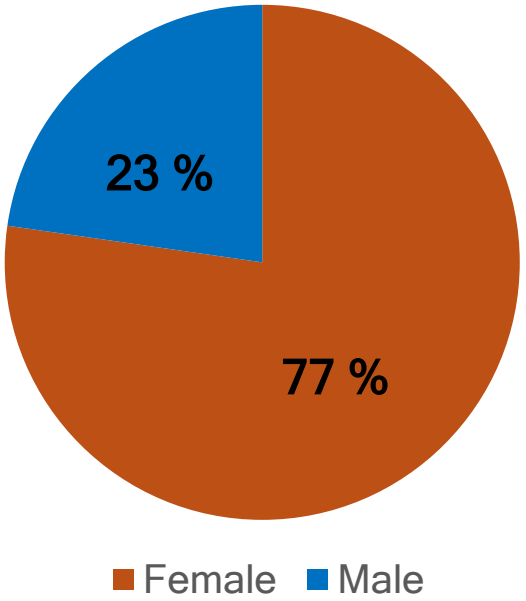


Participants

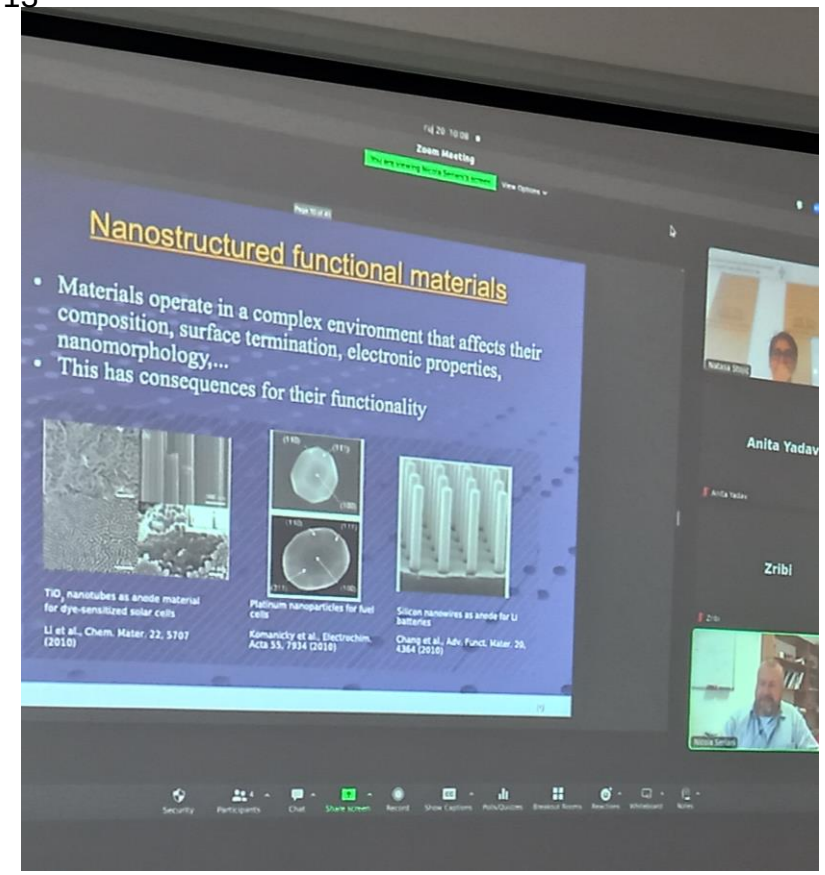
The 22 participants were from various scientific institutes in Tunisia!

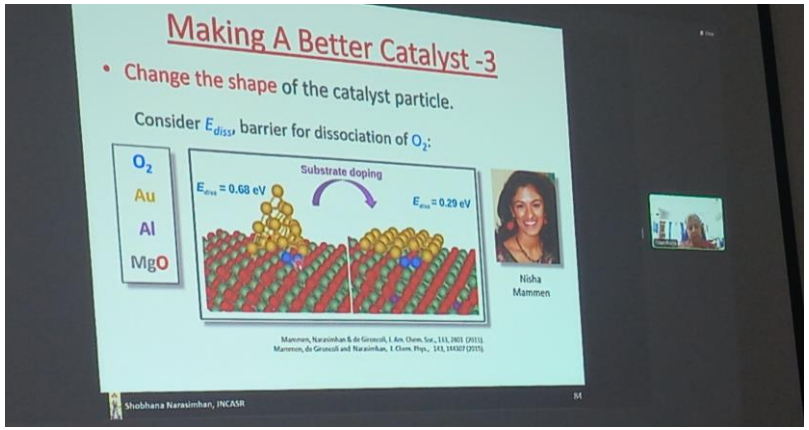


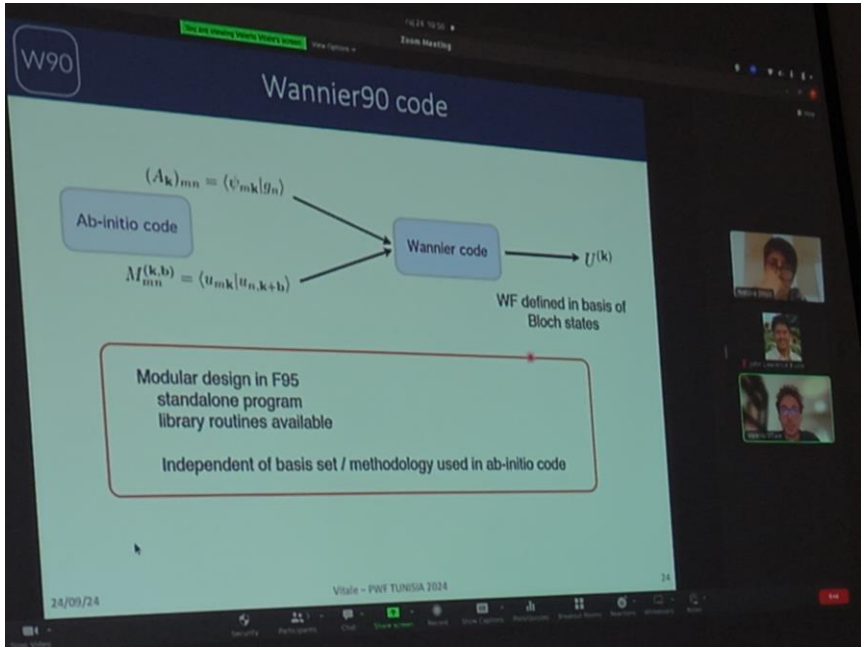
Highlights of the Activities

The morning sessions were dedicated to:

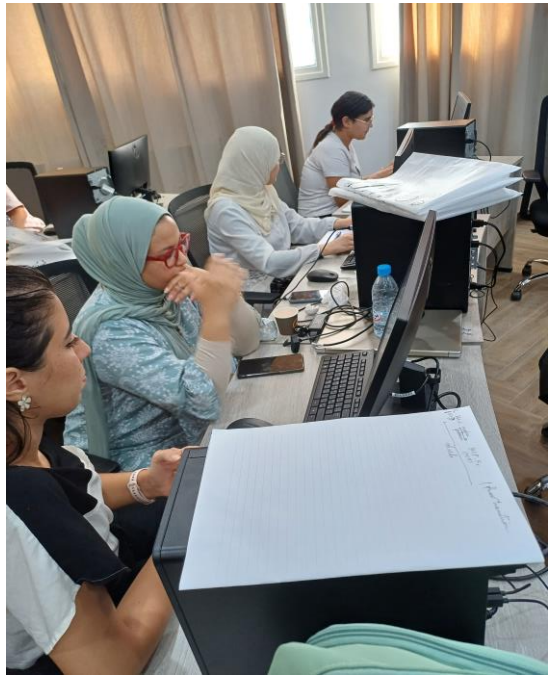
- Lectures on basic solid-state theory
- Introduction to density-functional theory
- Introduction to spintronics and renewable energy

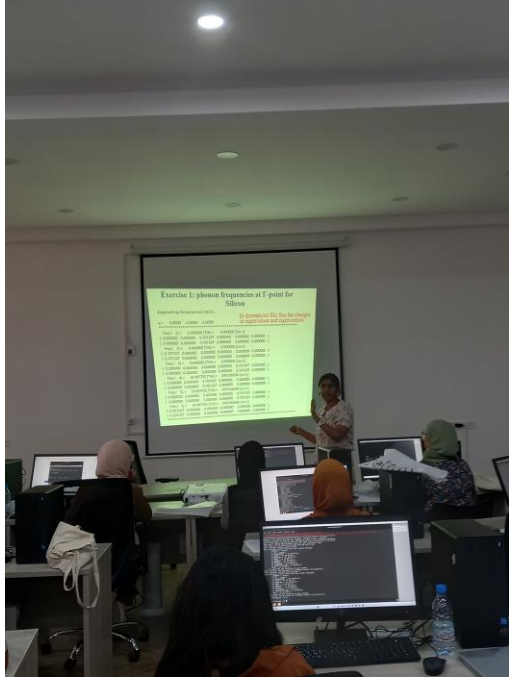


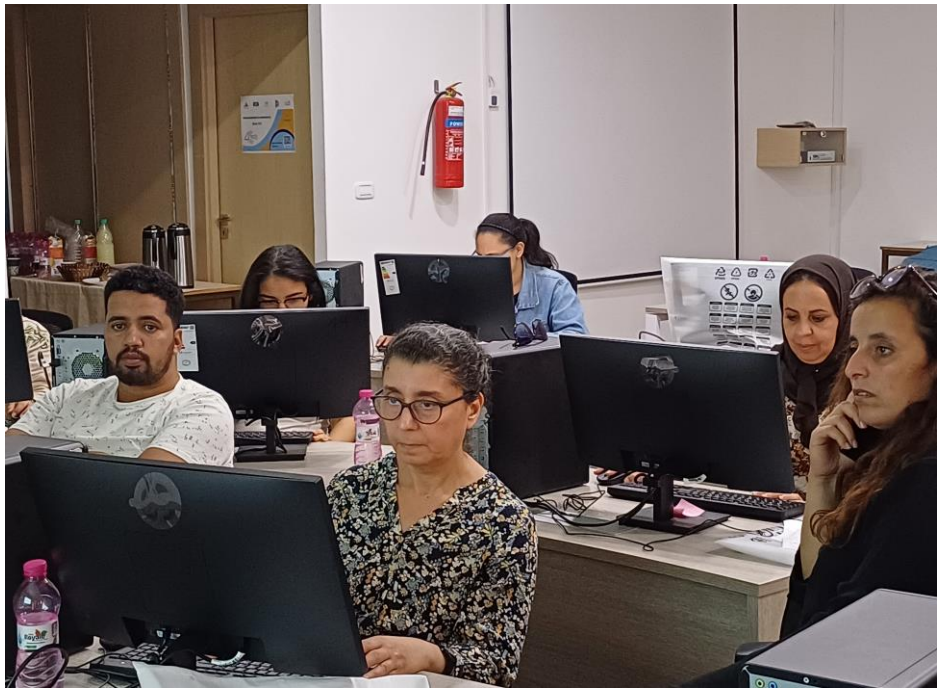




Online lectures on specific topics were given by experts in the field



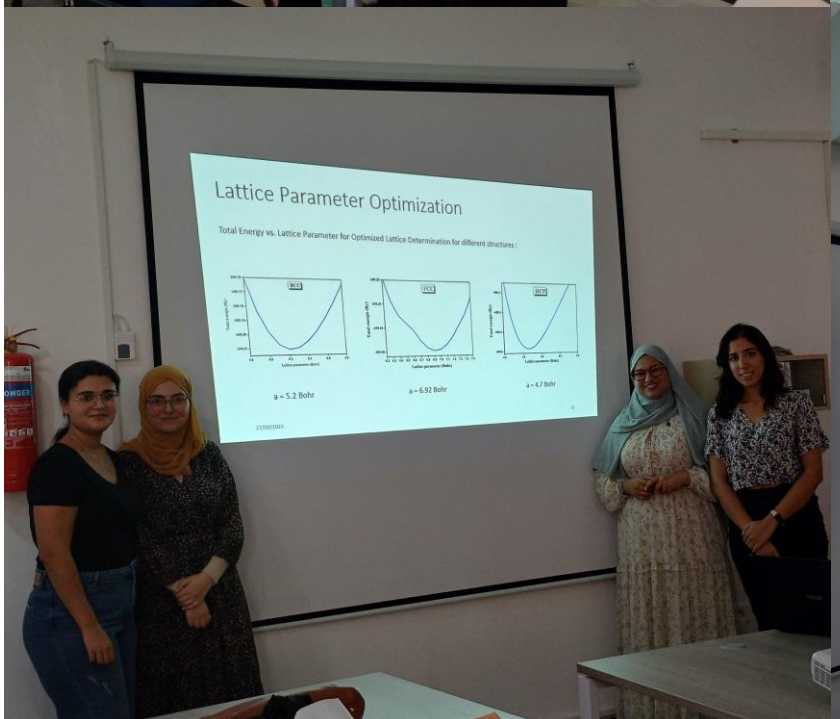




Long hands-on sessions were dedicated to first introducing DFT using Quantum Espresso and then applying it to more advanced examples

- 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