



Pole for Doctoral Studies
Center for Doctoral Studies
Sciences, Technologies, and Medical Sciences

ANNOUNCEMENT OF DOCTORAL THESIS DEFENSE



Ms. DNAYA Fatima Ezzahra

**Will present here research work with the aim of earning a
Doctorate**

Doctoral program: Engineering Science and Technology

Discipline: Physics

Specialty: Materials Science and Computational Physics

**On 23/07/2025 at 10H30 at the The Pr. Otman FILALI
MEKNASSI Conference Hall at the National School of Applied
Sciences in Tangier, UAE
Under the Theme**

**Multifaceted Understanding of Si-Nanostructures Properties
through DFT and TD-DFT**

Front of the jury composed of :

First Name & Last Name	Establishment	Designation
Pr. ACHAHBAR Abdelfattah	FS of Tetouan, UAE	President
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Pr. SOUBANE Driss	FP of Safi, UCD	Co-Supervisor
Pr. LAAZIZ Yassin	ENSA of Tangier, UAE	Supervisor

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Abstract



Silicon has served as the backbone of microelectronics for over half a century, owing to its unique electronic and physical properties, combined with mature and well-established fabrication techniques. While bulk silicon exhibits an indirect band gap that limits its optical efficiency, nanoscale silicon demonstrates enhanced radiative emission, making it a promising candidate for advanced photonic and photovoltaic applications.

In this thesis, we employ a multimodal computational approach to investigate the thermal dynamics structural stability and the optical properties of four hydrogen-passivated silicon nanostructures. We also explore possible configurations of surface-oxidized analogues to better understand the relationships among size, shape, and interface characteristics with the surrounding medium.

Our methodology integrates time-dependent density functional theory (TD-DFT) with *ab initio* molecular dynamics (AIMD), allowing for a comprehensive analysis of both the electronic structure and the structural evolution of Si zero-dimensional systems. This synergistic approach offers insight into the complex interplay between nanostructure geometry and dynamic behavior. Furthermore, we assess the optical response of these systems under external perturbations using TD-DFT with the turbo-Lanczos algorithm—a technique that achieves a balance between computational cost and accuracy. This enables the prediction of dynamic electronic excitations, which are critical for understanding and engineering light–matter interactions at the nanoscale.

Keywords: Nanostructures, Density Functional Theory (DFT), Time-dependent Density Functional Theory (TD-DFT), Silicon, Band-gap engineering.