

Títol	<i>Integrant Simulacions i Tractament de Dades Experimentals: Desvetllant la Resposta Mecànica dels Polielectròlits Dèbils a Nivell Molecular</i>
Title	Integrating Simulations and Experimental Data Treatment: Unveiling the Single-Molecule Mechanical Response of Weak Polyelectrolytes

Director	Marina I. Giannotti/Sergio Madurga
Departament	Ciència de Materials i Química Física
Universitat	Universitat de Barcelona
Tutor¹	

Curs	2023-24
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Summary²

The goal of this project is to study the mechanical response of weak polyelectrolytes at the single-molecule level to evaluate the interplay between charge regulation and mechanical stretching. Weak polyelectrolytes' charge can adapt in response to external stimuli (such as changes in pH, salt concentration, or electrostatic interaction with other charged species). This will be accomplished through single-molecule force spectroscopy (SMFS) using an atomic force microscope (AFM) under liquid environmental control. One of the main objectives is to design a protocol (performed by Python scripts) that involves aligning and normalizing multiple force-distance curves obtained from different experimental replicas. The comparison of the experimental curves will be conducted with the results of simulations using mechano-statistical theories, Monte Carlo (MC) computational methods, and/or all-atom molecular dynamics simulations.

Keywords³ Polyelectrolyte, stretching, force spectroscopy, atomic force microscopy (AFM), Monte Carlo, Molecular Dynamics

Breu descripció del projecte⁴

In nature, most relevant processes involve mechanical motion at the level of individual molecules. Furthermore, the macroscopic properties of polymeric materials are directly related to the chemical composition, structure, conformation and interactions at the molecular level. The nanomechanical study of macromolecules contributes to understanding fundamental aspects of the structure, mechanics and interaction of these molecules, whose elastic behavior is essential in both life sciences and materials science.

The mechanical response during stretching of weak polyelectrolytes is an area of mechano-chemistry that has not yet been explored. The charge of weak polyelectrolytes changes depending on the medium (pH, electrolytes...) and, therefore, it is expected that their mechanical properties do as well. The main objective of the project is to evaluate the relationship between charge regulation and the elastic properties of polyelectrolyte chains, using force spectroscopy experiments and comparison with computational simulations models.

The nanomechanical properties of polyelectrolytes are measured at the individual molecule level depending on their charge, regulated through variations in the aqueous medium (pH, ionic strength...). We use atomic force microscopy (AFM force spectroscopy), which allows us to record the force to which a polymer chain is subjected as it extends between two fixed points (to a surface and the tip of the AFM), in a liquid medium.

The student will carry out a bibliographic search on the study of macromolecules at an individual level using the proposed technique and, specifically, polyelectrolytes, as well as the models that are used today to describe the force-extension behavior in macromolecules/polyelectrolytes. For the study at the molecular level, Force-extension information of the polyelectrolytes deposited on defined surfaces from diluted solutions are collected through the use of atomic force microscopy, which allows the control and measurement of forces of the order of piconewtons (pN) and work in aqueous medium and controlled conditions (pH, electrolyte, etc.). In order to obtain reliable information, the obtained curves have to be processed in order to normalize and compare, by building master curves.

The TFM project aims to explore the mechanical response of weak polyelectrolytes at the single-molecule level, investigating the interplay between charge regulation and mechanical stretching. A key objective involves designing a Python-scripted protocol to align and normalize AFM force-distance curves obtained from diverse experimental replicas, ensuring consistency in data analysis. The protocol should enable systematic comparison of experimental curves. In addition, simulations based on mechano-statistical theories, Monte Carlo

computational methods, and/or all-atom molecular dynamics simulations will be performed to analyse the key interactions responsible for the variation of the different experimental conditions. This integrated approach aims at deepening our understanding of the mechanical behavior of weak polyelectrolytes.

¹Si el director no és un professor de la UB o de la UPC, caldrà assignar un tutor del TFM que designarà la Comissió Coordinadora del Màster.

²Aquest “summary” és el que apareixerà a la futura pàgina web dedicada al TFM. Procureu que sigui concís i entenedor (màx. 10 línies).

³Aquestes “keywords” no només són les que apareixeran al web sinó que ajudaran la Comissió Coordinadora del Màster a **assignar el projecte a un àrea concreta**.

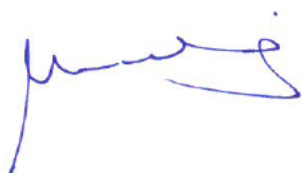
⁴Procureu ser concisos però proporcioneu prou informació per tal que l'estudiant i la Comissió Coordinadora del Màster es facin una idea prou acurada de en què consistirà el treball. **Indiqueu 3-6 publicacions de referència en la descripció del projecte per donar una idea dels fonament, metodologia, objectius, etc.**

Competències addicionals⁵ (opcional)

Observacions i comentaris

Per a la realització del treball pròpiament dit es preveu una dedicació d'unes quatre hores diàries durant cinc dies a la setmana, amb la opció de modificació de l'horari per poder adaptar-se millor a l'horari acadèmic de l'estudiant.

Tasques a desenvolupar ⁶		Cronograma (setmanes)																	
Tasca	Descripció	01	02	03	04	05	06	07	08	09	10	11	12	13	14	15	16	17	18
T01	Bibliografia (aprox. 50 h)	X	X	X				X	X										
T02	Aprenentatge del programari (aprox. 75h)		X	X	X	X	X												
T03	Simulacions (aprox. 150h)						X	X	X	X	X	X	X	X	X				
T04	Anàlisi i racionalització dels resultats (aprox. 100h)									X	X	X	X	X					
T05	Redacció de la memòria i preparar l'exposició (aprox. 100h)														X	X	X	X	X
T07	Script protocol for experimental data treatment of force-distance curves			X	X	X	X	X	X	X									
T08																			
T09																			
T10																			



Signatura: Marina Giannotti
(la directora del TFM)



Signatura: Sergio Madurga
(el codirector del TFM)

⁵ Enumereu breument qualsevol competència addicional a les competències genèriques enumerades en el Pla Docent del TFM (opcional).

⁶ Feu servir només les línies que calgui. Escolliu-les de manera que donin una idea aproximada de en què consistirà el treball i la seva distribució temporal.