

STudent REseArch Mobility Programme (STREAM)

Project proposal

Host University:

Université Paris-Saclay

Field (drop-down list):

Natural sciences, mathematics and statistics

Specified field, subject:

Molecular biophysics, Molecular modeling of intrinsically disordered proteins.

Research project title:

Molecular simulation of liquid-liquid phase separation of poly(amino acid)s.

Possible starting month(s):

Sep	Oct	Nov	Dec	Jan	Fev	Mar	Apr	May	Jun	Jul	Aug
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Possible duration in months:

1	2	3	4	5	6	7	8	9	10	11	12
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Exact starting and end dates will be discussed between the supervisor and the student

Date of validity: from 01/03/21 till 31/07/22

Suitable for students in: ☐ Bachelor level ☒ Master level

Universiteit
Leiden

Prerequisites: Background in physics, chemistry, or molecular biology.

Restrictions: None

Description (maximum 2,000 characters):

Liquid-liquid phase separation (LLPS) of proteins is a biological process involved in the formation of membrane-less organelles such as nucleoli or stress granules. Proteins that undergo LLPS are generally intrinsically disordered proteins with low complexity regions composed of repeats of short motifs that are rich in glycine, proline, serine, or threonine. Due to their extreme flexibility, the structures of these proteins and of their aggregates are difficult to be characterized at the atomic scale by experiments. In that context, the project aims at investigating the aggregation properties of poly(amino acid)s



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with low complexity sequence by using molecular modelling techniques. More specifically, the work will consist in performing molecular dynamics simulations of coarse-grained models of poly(amino acid)s and to study their aggregation and dissolution processes as a function of the temperature, the pH, and the ionic strength of the aqueous solution.

Research laboratory: BioCIS – Team FLUOPEPIT

Faculty and/or Department: Faculty of Pharmacy

Contact person, including position: Pr Tâp Ha-Duong

Contact email: tap.ha-duong@universite-paris-saclay.fr

Deadline for nomination to reach host university: 31/03/2022

Notification of admission given by the end of: 31/01/2022

Additional information: None

