



## NOTICE

### BASIC INFORMATION

Position available within the research project entitled: “Computational design of cationic polymers as gene delivery vectors”, code PN-III-P4-ID-PCE-2016-0474, Contract No. 36/2017

**Title\*:** ASSISTANT RESEARCHER – PHD STUDENT

### Offer Description\*:

Gene delivery is a cutting-edge research field, both experimentally and computationally. Cationic polymers (such as polyethylenimine) are among the most promising synthetic gene delivery vectors, used to condensate DNA to suitable sizes for penetrating into cells, protecting it from enzyme degradation, and finally releasing DNA with a view to its final processing inside the nucleus. The project aims to computationally design cationic polymers with geometrical structures and protonation distributions which optimize the entire delivery process.

Main objectives:

- Development of a novel fine-grained (CHARMM) force field (FF) for protonated PEI, rigorously derived from high-quality ab initio calculations.
- Fine-grained MD investigation of dynamic structuring of solvated PEI, in terms of gyration radius, end-to-end distance, persistence length, radial distribution functions, coordination, diffusion coefficients, and chain rigidity.
- Development of a novel coarse-grained (CG) FF for protonated PEI, mapping CHARMM residues to CG beads and adjusting the interaction parameters using as reference the atomistic FF and MD simulations.
- Fine- and CG MD investigations of DNA condensation under diverse conditions, aiming at enhanced efficiency of condensation/transfection processes.

### Researcher Profiles\*:

- |   |   |
|---|---|
| <input checked="" type="checkbox"/> First Stage Researcher (R1) | <input type="checkbox"/> Recognised Researcher (R2) |
| <input type="checkbox"/> Established Researcher (R3)            | <input type="checkbox"/> Leading Researcher (R4)    |

Research field \*:

Type of Contract\*:

Job Status \*:

Hours Per Week\*: 20

Application Deadline \*: 20 November 2017

Envisaged Job Starting Date: 1 December 2017

Is the job funded through a EU Research Framework Programme? \*

Is the Job related to staff position within a [Research Infrastructure](#)? (se bifează opțiunea)

How to Apply \*:

Internal Application form needed (.pdf files) (se bifează opțiunea, dacă este cazul)

## HIRING INFO & WORK LOCATION

Number of positions available\*: 1

Company/Institute\*: Babeş-Bolyai University

Department\*: Faculty of Physics / Department of Biomolecular Physics

## REQUIREMENTS

### Required Education Level

Main Research Field\*:

Level\*:

or

Main Research Field\*:

Level\*:

**Skills/Qualifications:**

PhD student in Physics or Chemistry.

Experience with numerical methods, scientific programming, and molecular dynamics simulations.

**Specific Requirements:**

**Required Languages**

Language \*

Level\*

Language \*

Level\*

**Required Research Experience**

Research Field \*

Years of Research Experience \*

or

Research Field \*

Years of Research Experience \*

**ADDITIONAL INFO**

**Website for additional job details:** *(câmp opțional)*

**Benefits:** *(câmp opțional)*

**Eligibility criteria:** *(câmp opțional)*

**Selection process:** *(câmp opțional)*

**Additional comments:** *(câmp opțional)*