



## NOTICE

POSITION: ASSISTANT RESEARCHER

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

APPLICATION DEAD-LINE: September 8, 2017

Project coordinator: Dr. Titus Beu, Professor (Theoretical and Computational Physics)

Work place: Babeş-Bolyai University,

Faculty of Physics / Department of Biomolecular Physics

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.

Nr. Job Position: 1

RESEARCH FIELDS:

PE – Physical Sciences and Engineering

- PE4 – Physical and Analytical Chemical Sciences (Physical chemistry of biological systems)



- PE3 – Condensed Matter Physics (Physics of biological systems)
- PE6 – Computer Science and Informatics (Bioinformatics, Biocomputing, and DNA and molecular computation)

Keywords: cationic polymers, polyethylenimine, gene delivery, force fields, molecular dynamics

CAREER STAGE: PhD student

RESEARCH PROFILE: Experience with numerical methods, scientific programming techniques, and molecular dynamics simulations.

REQUIREMENTS:

Required Educational Level	
DEGREE	Master degree or equivalent
DEGREE FIELDS	Physics, Chemistry, Chemical physics, Biophysics, Biochemistry, Bioinformatics
Required Research Experiences	
MAIN RESEARCH FIELDS	Computational physics, Molecular simulation methods, Electronic structure calculations, Numerical methods
RESEARCH SUBDOMAIN (area)	Molecular simulations of biophysical systems
Years of research experience	1
Required Languages	
LANGUAGE	English
LANGUAGE LEVEL	C1
Additional Requirements	
Good knowledge of numerical methods and programming languages (preferred C/C++ or Fortran).	

COMMENT/WEB SITE FOR ADDITIONAL JOB DETAILS: (type of contract, status, period, hours per week, etc)



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Fixed-term contract for a period of 27 months, starting October 1, 2017, with a work load of 40 hours/week.

<http://phys.ubbcluj.ro/~tbeu/index.html>

Additional details at: (contact person/project coordinator email address) [titus.beu@phys.ubbcluj.ro](mailto:titus.beu@phys.ubbcluj.ro)