Doctoral Position in Computational Chemistry

The research groups of Dr. J. Montenegro (http://www.javiermontenegrochemistry.com) (ERC-StG) and Dr. R. Garcia-Fandino (http://smmb.usc.es/rebeca) (Ramon y Cajal Researcher) are seeking for a **Doctoral candidate** with strong interest in the field of **Computational Molecular Dynamics Simulations** of supramolecular functional assemblies.

This is an excellent opportunity to join a cutting-edge research in Computational Chemistry and Chemical Biology and to work within the framework of international projects funded by the European Research Council (ERC) and the Human Frontiers Science Program (HFSP).

The general aim of the project is to understand, by means of **Molecular Dynamics Simulations** supported by experimental results, the **topological and structural motifs that govern the membrane translocation of peptides and proteins**, and to understand the basic principles behind the formation of the complex networks of nanofibers of the cellular cytoskeleton.

DESCRIPTION

Applying emerging computational methodologies, such as **Coarse-Grained-Molecular Dynamics** (CG-MD) and **All-atom-Molecular Dynamics** (AA-MD) MD accelerated with GPUs, different supramolecular architectures including applications in cellular delivery, molecular encapsulation and controlled delivery will be investigated.

The candidate will incorporate to an interdisciplinary group that actually combines a **strong computational approach** in the field membrane systems, with biochemical and biophysical characterization techniques of **membrane penetrating and bioactive molecules** as well as the polymerization and cross-linking of nanofibers in confined systems as cytoskeleton mimics.

REQUIREMENTS

We seek outstanding individuals with initiative, creativity and team-working ability and with a diploma in **Chemistry, Physics or Bioinformatics**.

Programming experience will be highly considered. Good communication skills and proficiency in written and spoken English are essential.

REFERENCES

"Hydrazone-modulated peptides for efficient gene transfection", I. Louzao, R. Garcia-Fandino, J. Montenegro. J. Mater. Chem. B **2017**, *5*, 4426-4434.

"Lipid bilayer membrane perturbation by embedded nanopores: a simulation study", R. Garcia-Fandino, A. Piñeiro, J. Trick, M. S. M. P. Sansom, ACS Nano **2016**, *10*, 3693-3701.

"Self-Assembly of Silver Metal Clusters of Small Atomicity on Cyclic Peptide Nanotubes" R. Garcia-Fandino, M. Cuerva, C. Vazquez-Vazquez, A. López-Quintela, J. Montenegro, J. R. Granja ACS Nano **2015**, *9*, 10834-10843.

STARTING DATE AND TERM

Spring 2018; starting date could be flexible. 3-4 years of contract (annual evaluation).

APPLICATIONS

Applicants must fill out the **Online application form** and they will receive an automatic acknowledgement (confirmation page). The final decision will be communicated via e-mail during April 2018.

Required data and pdf documents include BSc with all undergraduate numeric marks, and MSc (or title which provide access to PhD), as well as a brief CV (2 pages) and contact references.

In case of any problems, please contact us by mail (ciqus.jobs@usc.es; subject "PhD_ComputatChem1").

DEADLINE

Applications should be sent before **March, 28th**, 2018.