Πανεπιστήμιο Κύπρου

The Department of Physics at the University of Cyprus
is organizing a seminar on

Friday, 7 September 2018, time 12:30 p.m.

Room B228, Building 13, New Campus

Speaker:

Prof. Phanourios Tamamis

Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, United States

" Computational Design of Functional Amyloid Materials Binding to Ions and Compounds"

Amyloid materials constitute the basis for the design of novel functional materials[1-6]. Yet, experiments primarily rely on intuition to transform amyloid scaffolds into functional amyloid materials binding to ions or compounds. Thus, if the desired properties are hard to achieve, several peptide mutants need to be generated and tested experimentally, often with low success, making the procedure inefficient or nearly impossible. We present the first computational protocol for the design of functional amyloid materials, which combines MD simulations, an innovative computational optimization-based design model, big data analysis and free energy calculations[7]. Suitably selected amyloid peptide structures with termini not involved in the β-sheet amyloid core of the peptides (referred to by us as amyloid designable scaffolds which are inspired by Amyloid-β and the HIV-1 V3 loop[8]) are transformed into functional amyloid materials, by computationally designing their non-β-sheet residue positions to bind to certain ions or compounds, through mimicking "materialphore" models, representing how the specific ions or compounds bind to proteins according to experimentally resolved protein structures[7]. We applied this protocol for the design of amyloid materials capturing cesium ions from water[7]. Additionally we recently designed functional amyloid materials as drug carriers or antimicrobial compound carriers. The protocol can be advanced into a tool for the on demand design of novel amyloid materials of the future with promising applications in biomedicine and the environment.

1. Tamamis P et al. *Biophys J.* **2009**, 96, 5020-9.
2. Tamamis P et al. *J Phys Chem B.* **2009**, 113, 15639-47.
3. Tamamis P et al. *J Phys Chem B.* **2014**, 118, 1765-74.
4. Tamamis P et al. *Methods Mol Biol.* **2014**, 1216, 53-70.
5. Deidda G et al. *ACS Biomater Sci Eng.* **2017**, 3, 1404–1416.
6. Jonnalagadda SVR et al*. Mol. Syst. Des. Eng.,* **2017***,* 2, 321-335
7. Jonnalagadda SVR et al. *J Phys Chem B.* **2018**, 122, 7555−7568.
8. Kokotidou C et al. *FEBS Lett.* **2018**, 592, 1777-1788.

For more information, please contact:
Department of Physics, telephone: 22892826