Διακρίσεις Ι

Ο κ. **Αλεξιος Χατζηγούλας (Alexios Chatzigoulas)**, υποψήφιος διδάκτορας στο Ιδρυμα Ιατροβιολογικών Ερευνών της Ακαδημίας Αθηνών (ΙΙΒΕΑΑ), υπό την επίβλεψη της Δρ. Ζωής Κούρνια, έλαβε το δεύτερο βραβείο αναρτημένης ανακοίνωσης (poster PPO15) στα πλαίσια του 22nd European Symposium on Quantitative Structure-Activity Relationships (22nd Euro QSAR-2018), που διοργανώθηκε με επιτυχία στο Grand Hotel Palace στη Θεσσαλονίκη 16-20 Σεπτεμβρίου 2018. Η εργασία για την οποία βραβεύτηκε ο κ. Χατζηγούλας έχει τίτλο:

A web-based Crystallographic Tool for the Construction of Nanoparticles

22nd Euro QSAR Translation and Health Informatics: Implications for Drug Discovery
16-20 September 2018 / Thessaloniki, Greece

PP015

A WEB-BASED CRYSTALLOGRAPHIC TOOL FOR THE CONSTRUCTION OF NANOPARTICLES

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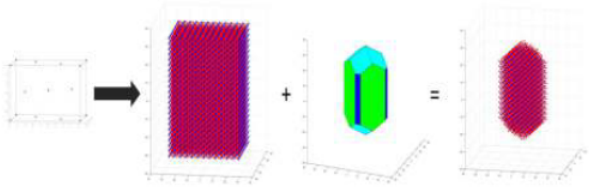
Nanoparticles have various applications in medicine, physics, optics, and electronics. Modeling nanoparticles is an essential first step to assess their capacity in different uses such as in energy storage or drug delivery [1]. However, creating an initial starting conformation for modeling and simulation is tedious, because every crystalline material grows with a different crystal habit and different symmetry in nature. That gave us the motivation to create the first web-based crystallographic tool, which creates nanoparticle models from any crystal structure guided by their preferred equilibrium shape in standard conditions according to Wulff morphology (crystal habit). The algorithm uses input from quantum mechanical calculations based on the Wulff construction. The Wulff construction employs energy minimization arguments to demonstrate that specific crystal planes are preferred over others, with their distance from the origin being proportional to their surface energy [2]. The input parameters for determining this equilibrium nanoparticle structure are the preferred growing planes as Miller indices, the energy of each plane, and the desired size of the nanoparticle. After inputting this data, the equilibrium shape is created with the following methodology. First, based on the crystallographic point group, the symmetric planes are produced based on the Miller indices, the fractional coordination system, and the lattice parameters. In this procedure, we place the origin on the negative side of these planes, and then we calculate the intersection points per three of the planes, discarding those that are on the positive side of at least one of the planes. Then, we obtain the faces of the equilibrium shape using the Quickhull algorithm [3] on the remaining intersection points, and the equilibrium shape is constructed by connecting these faces. The symmetric unit cell of the crystal structure is produced from the asymmetric one, using the lattice parameters and the symmetry operations of the crystallographic space group on the coordinates of the atoms again. Finally, the nanoparticle is constructed by replication of the unit cell across all three spatial directions, until the equilibrium shape is filled, and the coordinates of the atoms are output to the user in a .xyz and .pdb format and also visualized by JSmol. This tool has been implemented as a website using C++ and PHP and can be accessed and used at: http://nanocrystal.vi-seem.eu/CrystalTool.



The visualization of the algorithm's methodology.

References

[1] M. Patitsa, et al, Magnetic Nanoparticles Coated With Polyarabic Acid Demonstrate Enhanced Drug Delivery And Imaging Properties For Cancer Theranostic Applications, *Scientific Reports* (2017) 7, 775-782

[2] G. Barmparis, et al, Nanoparticle Shapes By Using Wulff Constructions And First-Principles Calculations, *Beilstein Journal Of Nanotechnology* (2015) 6, 361-368

[3] B. Barber, et al, The Quickhull Algorithm For Convex Hulls, *Acm Transactions On Mathematical Software (Toms)* (1995) 22(4), 469-483

Η Ελληνική Εταιρεία Φαρμακοχημείας συγχαίρει τον Κ. Χατζηγούλα και του εύχεται και νέες επιτυχίες.

Διακρίσεις ΙΙ

Η κ. Ερωφύλη Γιαννακοπουλου (Erofili Giannakopoulou), υποψήφια διδάκτορας στον Τομέα Φαρμακευτικής Χημείας του Τμήματος Φαρμακευτικής Ε.Κ.Π.Α. υπο την επίβλεψη του Επικ. Καθηγητή Γρηγόρη Ζωίδη, ήλθε πέμπτη στο διαγωνισμό φωτογραφίας που διοργανώθηκε στα πλαίσια του συνεδρίου EFMC/ISMC 2018. Από τις 71 φωτογραφίες που υποβλήθηκαν επελέγησαν 20 με πέμπτη τη φωτογραφία **Pink Martini** της Ερωφύλλης. Η Ελληνική Εταιρεία Φαρμακοχημείας συγχαίρει την κ. Γιαννακοπουλου και της εύχεται και νέες επιτυχίες

Ακολουθεί η ανακοίνωση της EFMC και η φωτογραφία Pink Martini

EFMC Photo Contest - Results of the votes !

The Communication Team is happy to announce the **20 pictures selected** for the second round of public voting, which will take place during the EFMC-ISMC 2018.

We were thrilled to receive **more than 1500 votes**, deciding between the 78 worthy candidates.

The selected pictures are:

- Combining education and research: Meet our team of future scientists - Stephanie Thee
- Paint my work - Susanna Zamolo
- Being a scientist in Coimbra - Raquel Martins Judite
- Just a tiny TLC plate might take all the lab to a sunny day at the seaside - Gulsah Bayraktar
- **Pink Martini - Erofili Giannakopoulou**
- Crystal Skyline - Lisa Barbaro
- Everyday struggle - Josipa Matic
- Dream as a Medicinal Chemist - Jean-Pierre Jourdan
- Metallic universe - Ruiz Belén Rubio
- Antibacterial: a melting contest - Davide Benedetto Tiz
- Triethylsalmiakki - Riccardo Provenzani
- Mass spectrometry lovers - Giovanna Baron
- Dreaming of Chemistry - David Cardoso
- Lab life - Caroline Lanthier
- Treating malaria: our goal on the horizon - Ana Sofia Martins Gomes
- Colors of condensations - Helena Gbelcová
- Eureka moment - Pedro Gonçalves
- Reflections - Gergo Mótyán

- A stinging legacy - Croci Federico
- Laboratory life 360° - Adriano Mollica

- **Pink Martini** - Erofili Giannakopoulou