

Name: FABIO MAVELLI

Institution: Department of Chemistry University Aldo Moro of Bari

Address: *Campus Universitario, Via Orabona, 4 – 70126 Bari IT*

Telephone: +39 080 544 2054

Cell Phone:

Email: fabio.mavelli@uniba.it

COURSE:

Physical Chemistry with Lab (Material Science - Bachelor Degree - Spring semester)

Modelling of Biological Systems (Industrial and Environmental Biotechnology Master Degree - Spring semester)

1. RESEARCH AND INTERNATIONAL ACTIVITY

Areas of scientific interest:

My research interests are mainly focused on the theoretical modelling of chemically reacting systems confined in micro-nano sized spaces. Two theoretical approaches are used for these kind of studies: (1) a deterministic approach, that requires the integration of sets of ordinary or partial differential equations; (2) a stochastic approach that requires to hand the Markov Master Equation or to mimic the system state dynamics by means of Monte Carlo simulations.

More recently we have also developed in our vet laboratory artificial compartmentalized systems (*protocells*) able to simulate the behaviour of real cells. Protocells consist of spherical giant unilamellar vesicles with sized in the range of 5-50 μm , where biomolecules (like enzymes, nucleic acid, membrane protein...) are encapsulated both in the internal aqueous core and/or in the lipid membrane. Examples of these studies can be found in the following selection of our articles:

1. Altamura E., *Highly oriented photosynthetic reaction centres generate a proton gradient in synthetic protocells*, PNAS in press.
2. K uchler A., Yoshimoto M., Luginb uhl S., Mavelli F., Walde P., *Enzymatic Reactions in Confined Environments*, Nature Nanotechnology 11, 409–420 (2016).
3. Mavelli F., Stano P., *Experiments and numerical modelling on the capture and concentration of transcription-translation machinery inside vesicles*. Artificial Life 21 (2015) 1–19.

4. Shirt-Ediss B., Ruiz-Mirazo K., Mavelli F., Sole RV., *Modelling Lipid Competition Dynamics in Heterogeneous Protocell Populations*, Scientific Reports 4, (2014), N.5675.
5. Walde P., Umakoshi H., Stano P., Mavelli F., *Emergent properties arising from the assembly of amphiphiles. Artificial vesicle membranes as reaction promoters and regulators*. Chemical Communications 50(71) (2014) 10177-10197.
6. Grotzky, A., Atamura, E., Adamcik, J.; Carrara, P., Stano, P., Mavelli, F. Nauser, T., Mezzenga, R., Schluter, A.D., Walde, P., *Structure and Enzymatic Properties of Molecular Dendronized Polymer–Enzyme Conjugates and Their Entrapment inside Giant Vesicles*. Langmuir 29, (2013) 10831-10840.
7. Mavelli F., Ruiz-Mirazo K., *Theoretical conditions for the stationary reproduction of model protocells*. Integrative Biology 5, (2013) 324-341.

International Activities:

2015 – Guest Editor of Special Issue "Protocells - Designs for Life", Life MDPI AG.

2015 – Chair of WIVACE 2015: International Workshop on Artificial Life and Evolutionary Computing, 22-24 of September 2016, Bari.

2015 – Local Organizer of COST-MEETING Action CM1304: Biomimetic Compartmentalized Chemical Systems, 24-25 of September 2016, Bari.

European projects:

2016-2017 EON Seed Grants "*Construction of minimal "cell mimicry" towards understanding of fundamental principles for origin of life*" dr. Soichiro Tsuda (Principal Investigator) School of Chemistry, University of Glasgow,

2013-2018 EU-COST Action CM1304: "Emergence and Evolution of Complex Chemical Systems " Italian Delegate in the Management Committee and team leader.

2013-2018 – Basque Government Grant (code: IT-590-13 Titled: "General Grant to consolidate the research group from the Basque Country"), prof. Alvaro Moreno (Principal Investigator) University of Basque Country.

Erasmus programme:

Chemistry – ULUDAĞ ÜNİVERSİTESİ - Rektörlük Uluslararası İlişkiler Ofisi 16059 Görükle/BURSA-TÜRKİYE.

2. ADDITIONAL INFORMATION (if need be)

In our group are welcomed students who are interested in developing theoretical methods for the description of the dynamics of complex reacting systems, but also students attracted by working experimentally in the implementation of artificial chemical systems that simulate the behaviour of real cells.