

SEMINAR

**Wednesday, 6th of April 2011 at 11:30 UPC Campus Nord, B4-212
(aula seminari)**

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Abstract

"Ionic transport through a biological nanochannel."

Understanding transport of charged solutes across transmembrane channels is a problem of paramount importance in biophysics, since it is crucial to regulate many cell functions [1]. An important property of biological nanochannels is their preference to the passage of either cations or anions through them, the so-called selectivity. New experiments on the selectivity of a biological nanochannel (the OmpF bacterial porin, a model channel) observe a reversal of selectivity in the presence of multivalent cations [2]. In my talk, I will discuss the results of new high-performance all-atom molecular dynamics simulations of the ionic transport across this biological nanochannel in the presence of electrolyte which provide an explanation for the experimental observations [3]. I will also discuss a method based on the calculation of first passage time quantities that was used to obtain macroscopic parameters which characterize the diffusive dynamics of the ions in the interior of the channel from the MD simulations' trajectories [4].

[1] B. Hille, *Ion Channels of Excitable Membranes* (Sinaure, Sunderland, 2001)

[2] A. Alcaraz et al., *Biophys. J.* 96, 56 (2009)

[3] M. Aguilera-Arzo, J. Faraudo, C. Calero, *Soft Matter* 6, 6079 (2010)

[4] C. Calero, J. Faraudo, M. Aguilera-Arzo, *Phys. Rev. E* 83, 021908 (2011)