Ciclo di incontri – Tavolo di discussione

Analyses of conduction and inactivation in K+ channels by Molecular Dynamics simulations

Simone Furini
Alma Mater Studiorum Università di Bologna - Bologna, Italy

Since the release of the first atomic structure of a K+-selective ion channel, back in 1998, Molecular Dynamics (MD) simulations have been one of the elected methods for analyzing the atomic mechanisms of conduction and selectivity. Nowadays, it is possible to simulate conduction in K+-channels at ion concentration and membrane potentials close to physiological conductions. Taking advantage of this possibility we estimated Markov State Models that describe conduction events in different potassium channels. We found that, at odds with the current paradigm, each K+-channel displays a characteristic permeation mechanism, with possible implications on both the channel conductance and its inactivation properties. In this seminar, I will discuss the current models of ion conduction across potassium channels, and how the dynamics of the pore region depends on the force field (CHARMM or AMBER) adopted in MD simulations.

Giovedì 27 Ottobre 2022 - Ore 11.00

Aula Didattica Palazzina E

Dipartimento di Ingegneria Meccanica e Aerospaziale - Via Eudossiana 18, Roma

Per dettagli contattare il Prof. Alberto Giacomello: alberto.giacomello@uniroma1.it

SAPIENZA UNIVERSITÀ DI ROMA

European Research Council
Established by the European Commission
Supporting top researchers from anywhere in the world