Salvatore M. Cosseddu

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EDUCATION

Doctor of Philosophy Biophysics/Biophysical Chemistry (PhD) April 2010 to date
School of Engineering and Centre for Scientific Computing,
University of Warwick, Coventry, UK

Thesis: *Structure and Dynamics of Protein in the Permeation, Selectivity and Gating of Potassium Ion Channels*.

Research description: Interdisciplinary joint research project between the Universities of Warwick and Lancaster, developed under the supervision of Dr Igor Khovanov (School of Engineering), Prof Mike P Allen (Department of Physics) and Prof Mark Rodger (Department of Chemistry), in collaboration with the Prof McClintock's group (Department of Physics, University of Lancaster), funded by EPSRC. I was associated with "Molecular Simulation" and "Biomedical" research groups. The research covered different fundamental features of K^+ ion channels: permeation, selectivity and inactivation processes. The research took advantage of the large-scale high performance computing resources of the Centre for Scientific Computing (University of Warwick).

Master of Science Physical Chemistry and Inorganic Chemistry (MSc, First-Class Honours) March 2010
Università degli Studi di Sassari, Sassari, Italy

Final project: One year project on developing a Kinetic Monte Carlo model to describe diffusion and reactivity in MFI-type zeolites.

Bachelor of Science Chemistry (BSc, First-Class Honours) March 2008
Università degli Studi di Sassari, Sassari, Italy
University of Nottingham, Nottingham, UK, six months within the Erasmus exchange programme

Final project: Six-months project on a Cellular Lattice Gas Automaton model to simulate reactivity in zeolites.

PROFESSIONAL EXPERIENCE

Researcher
Strong experience on investigation of

- Mechanisms and energetics of biological and non-biological processes;
- Structure-function relationship of protein;
- Highly-correlated non-linear dynamical properties of biological systems;
- Affinities between proteins and their substrates.

I have been involved in a joint research proposal on biological ion channels, submitted to EPSRC, between universities of Warwick and Lancaster in which I am a named researcher, PI Prof P.V.E. McClintock.

Laboratory demonstrator
University of Warwick, Coventry, UK
Laboratory demonstrator for Material Microstructure Laboratory and Statistical Mechanics.

SCIENTIFIC/TECHNICAL SKILLS

Broad interdisciplinary background

- Physical chemistry,
- Biophysics,
- Biochemistry,
- Molecular biology,
- Organic and inorganic chemistry,
- Pharmaceutical chemistry,
- Statistics,
- Classical and quantum mechanics
- Statistical mechanics,
- Thermodynamics,
- Scientific and high performance computing.

Technical skills

- Fine atomistic models (MD),
- State-of-the-art free-energy methods (MetaD, US)
- Statistical analyses.
- Coarse grained models (MC, KMC, BD)

COMPUTATIONAL SKILLS

Molecular simulations and statistical analysis

- NAMD,
- VMD,
- R,
- Gnuplot.

Languages and tools

Excellent knowledge:

- FORTRAN,
- Tcl,
- Bash,

Additional:

- Make and git (good),
- C, Matlab, Python (basic).

Office and graphics tools

- LaTeX (including Beamer),
- Emacs,
- Microsoft Office/OpenOffice,
- Gimp, Inkscape and Blender.

System administrator

- GNU/Linux (Debian and derived, Fedora, SUSE; I personally managed the Debian GNU/Linux workstations used during my PhD and MSc projects),
- Mac OS X,
- Windows OS.

COMMUNICATION SKILLS

- Pitch presentation and Poster presented to *2nd Annual CCP-BioSim Conference, Frontiers of Biomolecular Simulation*, 25 - 27 Mar 2013, Uni. of Nottingham, UK;
- Presentation of my research on *inactivation* in K^+ channels at CSC seminar, 11 Mar 2013, Uni. of Warwick, UK;
- Presentation of my research on *permeation* in K^+ channels at CSC seminar, 2 Dec 2013, Uni. of Warwick, UK;
- Presentations at postgraduate days of both CSC and School of Engineering;
- Poster presented to *South West Computational Chemists annual meeting 2013*, 24 Sep 2013, Uni. of Southampton, UK;
- Poster presented to *Beyond Molecular Dynamics: Long Time Atomic-Scale Simulations*, 26 - 29 Mar 2012, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany;
- I discussed and presented my works in meetings with various collaborators in which I learnt how to communicate with people with very different backgrounds;
- I presented my research and published papers in several occasions during regular meetings of the groups I was associated with;

PRIZES

- Awarded with the prize for the best talk at Centre for Scientific Computing's postgraduate day 2012.
- Poster selected by the School of Engineering in 2011 (still exposed) for advertising the different research activities of the department.

SELECTED ADDITIONAL CONFERENCES AND TRAINING

- *CCP5/RSC workshop Advances in Theory and Simulation of non-Equilibrium Systems*, 26 - 27 Jun 2013, Imperial College, UK;
- *CCP-BioSim workshop on Free energy methods for modelling of protein-ligand interactions*, 21 Nov 2012, Uni. of Southampton, UK;
- *Mathematical Modelling of Ion Channels Workshop*, 5 - 6 Sep 2011, St Anne's College, Oxford, UK;
- *Trends in protein biophysics: from in silico molecules to in vivo and vitro proteins*, 17 - 19 May 2011, Uni. of Warwick, UK;
- *CECAM/TCBG Computational Biophysics Workshop in Bremen*, 17 - 21 Oct 2011, Jacobs University, Germany;
- *IOP Condensed Matter and Materials Physics CMMP10*, 14 -16 Dec 2010, Uni. of Warwick, UK;
- *High Performance Scientific Computing* module, 2010/2011, Uni. of Warwick, UK;
- *CCP5 CECAM Methods in Molecular Simulation Summer School 2010*, 18 - 27 Jul 2010, Queens University Belfast, UK.

PUBLICATIONS

- S. M. Cosseddu, I. A. Khovanov, M. P. Allen, P. M. Rodger, D. G. Luchinsky, P. V. E. McClintock, *Dynamics of Ions in the Selectivity Filter of the KcsA Channel: Towards a Coupled Brownian Particle Description*, EJP-ST, 222, 2595-2605, 2013.
- S. M. Cosseddu, M. P. Allen, P. M. Rodger, I. A. Khovanov, *Highly-Coupled Network of Residues Underlying the Regulation of Conductivity in K^+ Ion Channels*, in preparation.
- S. M. Cosseddu, M. P. Allen, P. M. Rodger, I. A. Khovanov, *Mechanism and Energetic of C-type Inactivation in K^+ Ion Channels*, in preparation.
- S. M. Cosseddu, M. P. Allen, P. M. Rodger, I. A. Khovanov, *Energetics of Permeation and Selectivity of the Conductive State of K^+ Ion Channels*, in preparation.

MEMBERSHIPS

Associate member of the Institute of Physics.