

# RCB – Kolloquium

Donnerstag, 11. Juni 2026

14.00 Uhr

Neubau Biologie H 53



## Prof. Dr. Ulrich Zachariae

University of Dundee  
Faculty of Life Sciences

*Computational electrophysiology: Elucidating the function of Ca<sup>2+</sup> channels ion by ion*

Calcium is a fundamental biological signaling agent. The end point of a wide range of signals transduced through the cell membrane is an elevated Ca<sup>2+</sup> concentration in the cell; Ca<sup>2+</sup> ions thus have an impact on almost every aspect of cellular life.

Intracellular Ca<sup>2+</sup> concentrations are carefully controlled, and influx of Ca<sup>2+</sup> ions proceeds through highly regulated Ca<sup>2+</sup>-permeable channels.

We use computational electrophysiology, a biomolecular simulation technique that enables us to investigate Ca<sup>2+</sup> channel gating and permeation mechanisms “in real time” on the molecular level. Alongside an in-depth functional understanding, these simulations facilitate the identification of ligands with a desired effect on ion conduction, for example channel inhibitors as therapeutic drugs.

I will present our recent findings on members of the physiologically important Transient Receptor Potential (TRP) and Two-Pore Channel families, as well as the human CatSper Ca<sup>2+</sup> channel, whose function is essential for male fertility. Our simulations reveal how these channels are activated by various cues, how they enable ions to efficiently traverse the membrane, and how they achieve selectivity for Ca<sup>2+</sup> or competing cations. Furthermore, I will discuss a newly developed AI-based approach which allows us to generate activated, open channel conformations from closed state structures in the Protein Data Bank and the relevance of our work for the design of male contraceptives.

Host: Dr. Gregor Madej  
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