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It is a pleasure for me to wholeheartedly recommend the PhD. thesis of Josef Melcr for defense.

When Josef came to my group at the beginning of his PhD. studies we were pursuing a joint computational & experimental project aimed at developing voltage sensitive membrane fluorescence probes. Within this work we realized that there are two ways how to model a membrane potential – using an external electric field or by creating a charge imbalance at the two sides. We were not sure which method to use and Josef was very instrumental in resolving this problem. Namely, in a very nice computational study (published in JCTC) he showed that, at least for monovalent ions, the two methods give equivalent results, therefore one can safely utilize the simpler approach employing an external electric field.

When this study was completed I happened to hire a Finnish postdoc Samuli Ollila to help us develop accurate force fields for the description of interaction of biologically relevant ions with phospholipid membranes. We had a novel idea how to incorporate in a simple way electronic polarization effects, while Samuli had the computational machinery for force field refinement within his open collaboration web project NMRlipids. Josef quickly hopped on this train and the resulting collaboration proved to be very fruitful, resulting in three papers co-authored by him. The first one, published in PCCP, outlines the methodology

for obtaining ion-membrane interaction parameters by fitting to NMR order parameters employing the so called electrometer concept. The second paper (published in JPCB) presents accurate simulation results for binding of sodium and calcium ions to a zwitterionic phospholipid bilayer. The last study, which is currently finalized, deals with effects of negatively charged lipids on binding of cations to the membrane. On top of these papers, Josef also reported about his work in the form of contributed lectures or posters at several international conferences.

In conclusion, Josef did a very nice work on innovative simulations of ion-membrane systems with direct biological relevance (e.g., calcium signaling). During the course of his PhD. Josef learnt how to work efficiently and thus completed his postgraduate studies within five years despite being a dedicated and responsible father of two small daughters. I was very happy to have Josef in my group and I am sure that after defending his thesis he will flourish at his first postdoc position with a guru of coarse-grained simulations Prof. Siewert-Jan Marrink in Groningen.

Prof. Pavel Jungwirth