PERSONAL INFORMATION

Family name, First name: **Vacha, Robert**
Date of birth: 29th December 1980
ResearcherID, ORCID: D-1824-2012, 0000-0001-7610-658X
URL for web site: http://lcc.ncbr.muni.cz/~robert/

EDUCATION:

09/05 - 06/09 **Ph.D.** with **Pavel Jungwirth** at Faculty of Science, Charles University in Prague, Czech Republic - ***Molecular simulations of surfaces of aqueous solutions***

09/07 - 06/09 **International Max Planck Research School** for "Dynamical Processes in Atoms, Molecules and Solids" in Dresden, Germany

09/99 - 05/05 **MSc.** in Biophysics and Chemical Physics at Faculty of Mathematics and Physics, Charles University in Prague, Czech Republic
All exams passed with grade A - graduated with honor

POSITIONS:

04/16 – **Associate Professor** and **Researcher,** CEITEC (Central European Institute of Technology) and Faculty of Science at Masaryk University, Brno (Czech Republic)

10/11 –04/16 **Assistant Professor** and **Researcher,** CEITEC (Central European Institute of Technology) and Faculty of Science at Masaryk University, Brno (Czech Republic)

08/11 – 10/11 **Postdoctoral Research Associate,** group of Mikael Lund, Department of Chemistry, **Lund University** (Sweden): *Coarse-grained models of amyloids, Dynamic Monte Carlo (DMC) technique*

08/09 – 07/11 **Postdoctoral Research Associate**, group of Daan Frenkel, Department of Chemistry, **University of Cambridge** (UK): *Coarse-grained models of phospholipid membranes and proteins MD and MC*

FELLOWSHIPS:

06/10 – 08/11 **Junior Research Fellowship** at Churchill College, Cambridge Highly competitive research fellowship - few postdoc positions within the whole University of Cambridge per year

11/08 - 12/08 **Fellowship** in group of Nobuyuki Matubayasi at Institute for Chemical Research, **Kyoto University** in Japan: *Investigation and application of free energy calculations*

09/07 - 09/07 **Fellowship** in group of **Max Berkowitz** at University of North Carolina, USA

07/06 - 08/06 **Fellowship** in group of **Rainer Böckmann** at University of Saarland, Germany

TEACHING ACTIVITIES AND MENTORING:

2017 - **Lecturing** – *Problems and issues of molecular modelling* C9926 Masaryk University, Czech Republic

2016 - **Lecturing** – *Seminar of molecular modelling* F1170 Masaryk University, Czech Republic

2015 - **Lecturing** - *Physics of biopolymers* F8510 Masaryk University, Czech Republic

2013 - **Lecturing** - *Interactions of proteins and membranes – introduction to soft matter* NBCM147, Charles University, Prague, Czech Republic

2012 - **Lecturing** - *Introduction to soft matter models of membranes and proteins* C9925, Masaryk University, Czech Republic

2010 - 2011 **Supervisions** of *Thermodynamics and Kinetics* at Churchill College, Cambridge (3 small groups of three 1st year students)

2010 - 2011 **Mentoring** 5 students (2 Ph.D. and 3 MSc.)

2009 - 2010 **Supervisions** of *Statistical Mechanics* at Chemistry Department, University of Cambridge (small group teaching of three 3rd year students)

2007 - 2008 **Assistant** teacher of *Classical molecular dynamics* at Faculty of Mathematics and Physics, Charles University in Prague

2006 - 2007 **Assistant** teacher of *Classical and quantum molecular dynamics* at Faculty of Mathematics and Physics, Charles University in Prague

GRANTS:

2017 - 2020 Czech Science Foundation grant (**GACR**) – PI, Amphiphilic Peptides at Phospholipid Membranes, 3 years (180 000 EUR)

2016 - 2019 European Regional Development Fund (**ERDF**) Program Interreg V-A Austria-Czech Republic – co-applicant, Protein Dynamic Center (PDC), 3 years (898 000 EUR)

2014 - 2016 Czech Science Foundation grant (**GACR**) – PI, Self-assembly of patchy spherocylinders, 3 years (160 000 EUR)

2008 Japan Society for the Promotion of Science (**JSPS**) - fellowship grant at Institute for Chemical Research, Kyoto University, Japan, 2 months, Investigation and application of novel free energy calculations (3 300 EUR)

2008 Grant Agency of Charles University **GAUK** – PI, 1 year grant, Czech Republic Creation on investigation of mixed phospholipid membrane with atomistic resolution by means of computer simulations (4 600 EUR)

INVITED LECTURES (selected):

2016 Organizing Molecular Matter - A soft matter symposium, Lund, Sweden

2015 CEITEC/ICRC Annual Conference, Brno, Czech Republic

2013 TAPPO workshop, Levi, Finland

2012 CECAM workshop - Design of Self-assembling Materials, Vienna, Austria

2012 Telluride Science Research Center - Protein and Peptide Interactions in Cellular Environments, Telluride, CO, USA

2011 ACS national meeting, Denver, USA

2010 Hofmesiter fest – Hofmeister series and ion specificity, Prague, Czech Republic

AWARDS:

2014 Best talk of early stage researcher – CECAM workshop

2013 International travel award from Biophysical Society

06/10 – 08/11 **Junior Research Fellowship** at Churchill College, Cambridge Highly competitive and prestigious research fellowship – a dozen postdoctoral positions are offered per year within the whole of the University of Cambridge

2010 **Bolzano Prize** in natural sciences - Charles University in Prague – awarded to the two best Ph.D. theses in the natural sciences at Charles University each year

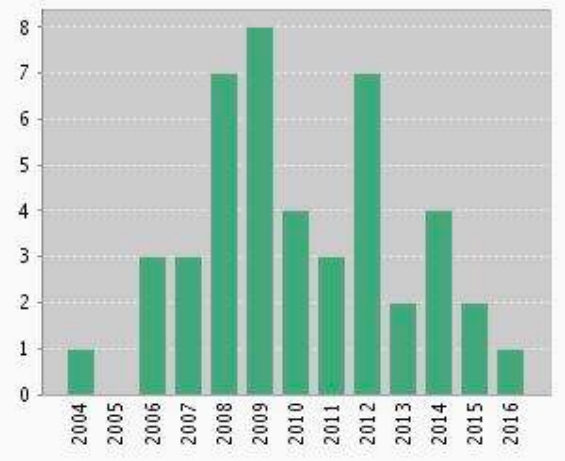
09/99 – 06/04 Scholarship for the 50 best students in each year (about 10% of all students)

PUBLICATIONS:

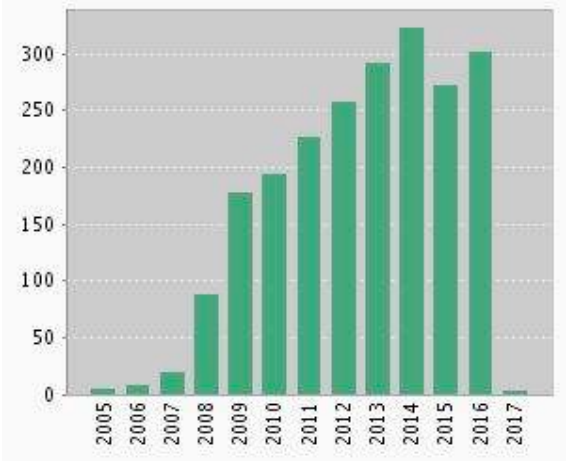
I have published 41 peer-reviewed articles, one book chapter and three editorial comments in major international journals that have attracted 2000+ citations (excluding self-citations according to ISI Web of Science in Jan 2017), yielding an H-index of 26. These publications include PNAS, Nano letters, ACS Nano, JACS, Angewandte Chemie, and Accounts of Chemical Research. I am the corresponding author of 10 articles. I review 6-12 paper a year.

Publication record of the PI according to the ISI Web of Science in Jan 2017:

Published Items in Each Year



Citations in Each Year



COLLABORATIONS:

Jiří Nováček – CEITEC MU core facility Cryo-electron Microscopy and Tomography – protein-protein interactions (experiment planned together in Interreg grant 2016-2019)

Pavel Plevka – CEITEC MU – cryoEM, protein-protein interactions in virus capsids

Vítězslav Bryja – Masaryk University – fluorescence, FRET, post-translational modifications, biocheistry – Dishavelled protein (DVL)

Martin Hof – Institute of physical chemistry J. Heyrovsky AVČR– fluorescence spectroscopy, FRET, FCC, CD, leakage assay – interaction of peptides and membranes

Thomas Leonard – Max Perutz Labs (Austria) – x-ray, NMR – structure determination and membrane interaction of protein kinases (PKD)

Burkhard Bechinger – Strasburg University (France) – solid state NMR – peptide orientation at membranes

Mikael Lund – Lund University (Sweden) – Monte-Carlo, coarse grained models, small angle X-ray, peptides and proteins interactions in solution and at membrane

Sara Linse and Emma Sparr – Lund University (Sweden) – fluorescence, SPR, QCM - aggregation of peptides and their interaction with membranes (Abeta)

Peter Jönsson and Klas Flärdh – Lund University (Sweden) – fluorescence, post-translational modification, small angle x-ray, PCR, ultracentrifugation – DivIVA protein

Julian Naglik – King's College, London (UK) – peptide purification, biochemistry, CD, leakage assay – Candidalysin peptide

Summary of academic and other professional experience

Experience:

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2016 - 2019 Interreg V-A Austria-Czech Republic grant from European Regional Development Fund (**ERDF**) Program, Protein Dynamic Center (PDC), 3 years, co-applicant (responsible from modeling part), 898 000 EUR

2014 - 2016 Standard grant from Czech Science Foundation (**GACR**), Self-assembly of amphiphilic peptides with helical character, 3 years, PI, 160 000 EUR

2008 Fellowship grant at Institute for Chemical Research at Kyoto University from Japan Society for the Promotion of Science (**JSPS**), Investigation and application of novel free energy calculations, 2 months, PI, 3 300 EUR

2008 Student grant from Grant Agency of Charles University **GAUK**, Creation on investigation of mixed phospholipid membrane with atomistic resolution by means of computer simulations, 1 year, PI, 4 600 EUR

Research papers:

40. Amaro, M.; Sachl, R.; Aydogan, G.; Mikhalyov, I.I.; **Vácha, R.**; Hof, M.: GM1 Ganglioside Inhibits beta-Amyloid Oligomerization Induced bySphingomyelin**.** *Angewandte Chemie International Edition* **2016**, 55, 1-6, IF= 10.777

39. Kabelka, I.; **Vácha, R.**: Optimal conditions for opening of membrane pore by amphiphilic peptides. *The Journal of Chemical Physics* **2015**, 143, 243115, IF= 2.952

38. Schubertová, V.; Martinez-Veracoechea, F.J.; **Vácha, R.**: Influence of ligand distribution on uptake efficiency. *Soft Matter* **2015**, 11, 2726-2730, IF=4.029

37. **Vácha, R.**; Linse, S.; Lund, M.: Surface Effects on Aggregation Kinetics of Amyloidogenic Peptides. *Journal of American Chemical Society* **2014**, 136 (33), 11776-11782, IF=11.444

36. **Vácha, R.**; Frenkel, D.: Stability of Bicelles: A Simulation Study. *Langmuir* **2014**, 30 (15), 4229-4235, IF=4.384

35. **Vácha, R.**; Frenkel, D.: Simulations Suggest Possible Novel Membrane Pore Structure. *Langmuir* **2014**, 30 (5), 1304-1310, IF=4.384

34. Shi, Q.; Bergquist, K.-E.; Huo, R.; Li, J.; Lund, M.; **Vácha, R.**; Sundin, A.; Butkus, E.; Orentas, E.; Warnmark, K.: Composition- and Size-Controlled Cyclic Self-Assembly by Solvent and C60-Responsive Self-Sorting. *Journal of American Chemical Society* **2013**, 135 (40), 15263-15268, IF=11.444

33. Stenqvist, B.; Thuresson, A.; Kurut, A.; **Vácha, R.**; Lund, M.: Faunus - a flexible framework for Monte Carlo simulation. *Molecular Simulation* **2013**, 39(14-15), 1233-1239, IF=1.119

32. **Vácha, R.**; Martinez-Veracoechea, F.J.; Frenkel, D.: Intracellular Release of Endocytosed Nanoparticles Upon a Change of Ligand-Receptor Interaction. *ACS Nano* **2012**, 6 (12), 10598-10605, IF=12.033

31. Bieler, N.S.; Knowles, T.P.J.; Frenkel, D.; **Vácha, R.**: Connecting Macroscopic Observables and Microscopic Assembly Events in Amyloid Formation Using Coarse Grained Simulations. *PLoS Computational Biology* **2012**, 8 (10), e1002692, IF=4.867

30. **Vácha, R**.; Roke; S.: Sodium Dodecyl Sulfate at Water-Hydrophobic Interfaces: A Simulation Study. *Journal of Physical Chemistry B* **2012**, 116 (39), 11936-11942, IF=3.377

29. Vazdar, M.; Pluharová, E.; Mason, P.E.; **Vácha, R**.; Jungwirth, P.: Ions at Hydrophobic Aqueous Interfaces: Molecular Dynamics with Effective Polarization. *Journal of Physical Chemistry Letters* **2012**, 3, 2087-2091, IF=6.687

28. **Vácha, R.**; Marsalek, O.; Willard, A.P.; Bonthuis, D.J.; Netz, R.R.; Jungwirth, P.: Charge Transfer between Water Molecules As the Possible Origin of the Observed Charging at the Surface of Pure Water. *Journal of Physical Chemistry Letters* **2011**, 3, 107-111, IF=6.687

27. **Vácha, R.**; Martinez-Veracoechea, F.J.; Frenkel, D.: Receptor-Mediated Endocytosis of Nanoparticles of Various Shapes. *Nano Letters* **2011**, 11 (12), 5391-5395, IF=12.940

26. **Vácha, R.**; Frenkel, D.: Relation between Molecular Shape and the Morphology of Self-Assembling Aggregates: A Simulation Study. *Biophysical Journal* **2011**, 101, 1432-1439, IF=3.832

25. **Vácha, R.**; Rick, S.W.; Jungwirth, P.; de Beer, A.G.F.; de Aguiar, H.B.; Samson, J.-S.; Roke, S.: The Orientation and Charge of Water at the Hydrophobic Oil Droplet–Water Interface. *Journal of American Chemical Society* **2011**, 133 (26), 10204-10210, IF=11.444

24. Pospíšil, M.; Kovár, P.; **Vácha, R.**; Svoboda, M.: Study of the betulin molecule in a water environment; ab initio and molecular simulation calculations. *Journal of Molecular Modeling* **2011**, 1-10, IF=1.867

23. Wolff, W.; McKenna, J.; **Vácha, R.**; Zohrabi, M.; Gaire, B.; Carnesa, K.D.; Ben-Itzhak, I.: Three-dimensional energy profile measurement of a molecular ion beam by coincidence momentum imaging compared to a retarding field analyzer. *Journal of instrumentation* **2010**, 5, P10006, IF=1.526

22. **Vácha, R.**; Jurkiewicz, P; Petrov, M.; Berkowitz, M.L.; Böckmann, R. A.; Barucha-Kraszewska, J.; Hof, M.; Jungwirth, P.: Mechanism of Interaction of Monovalent Ions with Phosphatidylcholine Lipid Membranes. *Journal of Physical Chemistry B* **2010**, 114 (29), 9504-9509, IF=3.377

21. Lund, M.; Jagoda-Cwiklik, B.; Woodward C.E.; **Vácha, R.**; Jungwirth, P.: Dielectric Interpretation of Specificity of Ion Pairing in Water. *Journal of Physical Chemistry Letters* **2010**, 1(1), 300-303, IF=6.687

20. Ottosson, N.; **Vácha, R.**; Aziz, E. F.; Pokapanich, W.; Eberhardt, W.; Svensson, S.; Öhrwall, G.; Jungwirth, P.; Björneholm, O.; Winter, B.: Large variations in the propensity of aqueous oxychlorine anions for the solution/vapor interface. *Journal of Chemical Physics* **2009**, 131, 124706, IF=3.122

19. Winter, B.; Faubel, M.; **Vácha, R.**; Jungwirth, P.: Behavior of hydroxide at the water/vapor interface. *Chemical Physics Letters* **2009**, 474, 241-247, IF=1.991

18. Heyda, J.; Pokorna, J.; Vrbka, L.; **Vácha, R.**; Jagoda-Cwiklik, B.; Konvalinka, J.; Jungwirth, P.; Vondrasek, J.: Ion specific effects of sodium and potassium on the catalytic activity of HIV-1 protease. *Physical Chemistry Chemical Physics* **2009**, 11, 7599-7604, IF=4.198

17. **Vácha, R.**; Berkowitz, M. L.; Jungwirth, P.: Molecular Model of a Cell Plasma Membrane with an Asymmetric Multicomponent Composition: Water Permeation and Ion Effects. *Biophysical Journal* **2009**, 96(11), 4493-4501, IF=3.832

16. **Vácha, R.**; Megyes, T.; Bako, I.; Pusztai, I.; Jungwirth, P.: Benchmarking polarizable molecular dynamics simulations of aqueous sodium hydroxide by diffraction measurements. *Journal of Physical Chemistry A* **2009**, 113 (16), 4022-4027, IF=2.775

15. **Vácha, R.**; Siu, S. W. I.; Petrov, M.; Böckmann, R. A.; Barucha-Kraszewska, J.; Jurkiewicz, P.; Hof. M.; Berkowitz, M. L.; Jungwirth, P.: Effects of alkali cations and halide anions on the DOPC lipid membrane. *Journal of Physical Chemistry B* **2009**, 113 (26), 7235-7243, IF=3.377

14. Vlachy, N.; Jagoda-Cwiklik, B.; **Vácha, R.**; Touraud, D.; Jungwirth, P.; Kunz, W.: Hofmeister series and specific interactions of charged headgroups with aqueous ions. *Advances in Colloid and Interface Science* **2009**, 146, 42, IF=8.636

13. Aziz, E. F.; Ottosson, N.; Eisebitt, S.; Jagoda-Cwiklik, B.; **Vácha, R.**; Jungwirth, P.; Winter, B.: Cation-specific interactions with carboxylate in amino acid and acetate aqueous solutions: X-ray absorption and ab initio calculations. *Journal of Physical Chemistry B* **2008**, 112, 12567-12570, IF=3.377

12. **Vácha, R.**; Horinek, D.; Berkowitz, M. L.; Jungwirth, P.: Hydronium and hydroxide at the

interface between water and hydrophobic media. *Physical Chemistry Chemical Physics* **2008**, 10, 4975-4980, IF=4.198

11. **Vácha, R.**; Zangi, R.; Engberts, J. B. F. N.; Jungwirth, P.: Water Structuring and Hydroxide Ion Binding at the Interface between Water and Hydrophobic Walls of Varying Rigidity a nd van der Waals Interactions. *Journal of Physical Chemistry C* **2008**, 112 (20), 7689-7692, IF=4.835

10. **Vácha, R.**; Cwiklik, L.; Rezac, J.; Hobza, P.; Jungwirth, P.; Valsaraj, K.; Bahr, S.; Kempter, V.: Adsorption and Heterogeneous Reactions of Aromatic Hydrocarbons at Environmental Aqueous Surfaces. *Journal of Physical Chemistry A* **2008**, 112 (22), 4942-4950, IF=2.775

9. Siu, S. W. I; **Vácha, R.**; Jungwirth, P.; Böckmann, R. A.: Biomolecular simulations of membranes: Physical properties from different force fields. *Journal of Chemical Physics* **2008**, 128, 125103, IF=3.122

8. Lund, M.; **Vácha, R.**; Jungwirth, P.: Specific Ion-Binding to Macromolecules: Effects of Hydrophobicity and Ion Pairing. *Langmuir* **2008**, 24(7), 3387-3391, IF=4.384

7. Jagoda-Cwiklik, B.; **Vácha, R.**; Lund, M.; Srebro, M.; Jungwirth, P.: Ion pairing as a possible clue for discriminating between sodium and potassium in biological and other complex environments. *Journal of Physical Chemistry B* **2007**, 111, 14077-14079, IF=3.377

6. **Vácha, R.**; Buch, V.; Milet, A.; Devlin J.P.; Jungwirth, P.: Autoionization at the surface of neat water: is the top layer pH neutral, basic, or acidic? *Physical Chemistry Chemical Physics* **2007**, 34, 4736-4747, IF=4.198

5. Buch, V.; Milet, A.; **Vácha, R.**; Jungwirth, P.; Devlin J.P.: Water surface is acidic. *Proceedings of the National Academy of Sciences of the United States of America* **2007**, 107 (18), 7342-7347, IF=9.809

4. Vrbka, L.; Vondrášek, J.; Jagoda-Cwiklik, B.; **Vácha, R.**; Jungwirth, P.: Quantification and rationalization of the higher affinity of sodium over potassium to protein surfaces. *Proceedings of the National Academy of Sciences of the United States of America* **2006**, 103 (42), 15440-15444, IF=9.809

3. **Vácha, R.**; Jungwirth, P.; Chen, J.; Valsaraj, K.: Adsorption of polycyclic aromatic hydrocarbons at the air-water interface: Molecular dynamics simulations and experimental atmospheric observations. *Physical Chemistry Chemical Physics* **2006**, 8 (38), 4461-4467, IF=4.198

2. Minofar, B.; **Vácha, R.**; Wahab, A.; Mahiuddin, S.; Kunz, W.; Jungwirth, P.: Propensity for the air/water interface and ion pairing in magnesium acetate vs magnesium nitrate solutions: Molecular dynamics simulations and surface tension measurements. *Journal of Physical Chemistry B* **2006**, 110 (32), 15939-15944, IF=3.377

1. **Vácha, R.**; Slavicek, P.; Mucha, M.; Finlayson-Pitts, B. J.; Jungwirth, P.: Adsorption of atmospherically relevant gases at the air/water interface: Free energy profiles of aqueous solvation of N_2, O_2, O_3, OH, H_2O, HO_2, and H_2O_2. *Journal of Physical Chemistry A* **2004**, 108, 11573-11579, IF=2.775

Review paper:

R1. Berkowitz, M.L. and **Vácha, R**.: Aqueous Solutions at the Interface with Phospholipid Bilayers. *Accounts of Chemical Research* **2012**, 45 (1), 74-82, IF=24.348

Editorial material:

E1. **Vácha, R.**; Horinek, D.; Buchner, R.; Winter, B.; Jungwirth, P.: Comment on "An explanation for the charge on water's surface" by A. Gray-Weale and J. K. Beattie, Phys. Chem. Chem. Phys., 2009, 11, 10994. *Physical Chemistry Chemical Physics* **2010**, 12 (42), 14362-14363, IF=4.198

E2. Winter, B.; Faubel, M.; **Vácha, R.**; Jungwirth, P.: Reply to comments on Frontiers Article 'Behavior of hydroxide at the water/vapor interface'. *Chemical Physics Letters* **2009**, 481, 19-21, IF=1.991

E3. **Vácha, R.**; Buch, V.; Milet, A.; Devlin J.P.; Jungwirth, P.: Response to Comment on Autoionization at the surface of neat water: is the top layer pH neutral, basic, or acidic? by J. K. Beattie, Phys. Chem. Chem. Phys., 2007, 9, DOI : 10.1039/b713702h. *Physical Chemistry Chemical Physics* **2008**, 10 (2), 332-333, IF=4.198

Book chapter:

Vácha, R.; Uhlig, F.; Jungwirth, P.: Charges at aqueous interfaces: development of computational approaches in direct contact with experiment. *Advances in Chemical Physics* **2014**, 155, 69-95

Training and research career

I did my undergraduate studies at **Faculty of Mathematics and Physics, Charles University in Prague**, where I studied Physics major with specialization on Chemical physics and biophysics. I passed all the exams with grade A, regularly obtained study scholarship (10% best students), and graduated with honor in 2005. I continued under supervision of **Pavel Jungwirth** for PhD at **Faculty of Science, Charles University in Prague** with specialization: Simulation of chemical properties of nano- and biostructures. I participated in the **International Max Planck Research School** and completed **a number of international fellowships.** In 2009, I defended thesis with title "Molecular simulations of surfaces of aqueous solutions", which was awarded **Bolzano prize** (awarded to the two best Ph.D. theses in the natural sciences at Charles University each year). The research was focused on behaviour of small molecules and ions at water/air and water/membrane interfaces. We found that the pure water surface is not ion free and hydronium ions are more abundant at the top most water layer than hydroxide anions. Moreover, we determined the mechanism by which different ions adsorb to the phospholipid membranes. I used *ab initio* and all-atom models together with molecular dynamics techniques. The results were published in 16 peer review papers in renowned international journals including **two Proceedings of the National Academy of Sciences** (**PNAS, IF:9.681**). Subsequently, I was invited to write a review without my PhD advisor in **Accounts of Chemical Research** (**IF:24.348**).

For postdoc I moved to work with Daan Frenkel at Chemistry Department, **University of Cambridge**, where I learned to develop coarse-grained models and use Monte Carlo techniques. I continued research of phospholipid membranes with focus on their interaction with amphiphilic molecules and nanoparticles. I was awarded **Junior Research Fellowship** (Churchill College), which is highly competitive and prestigious award given only to **a dozen of postdocs from the whole University of Cambridge per year**. My second postdoc was with Mikael Lund at **Lund University**, where I learned more about coarse-grained models of proteins. Results were published in a number of prestigious journals including **Nano Letters (IF:12.940), ACS Nano (IF:12.033), and Journal of the American Chemical Society (JACS, IF:11.444**).

In 2011, I returned to Czech Republic to CEITEC and Faculty of Science, MU. Since then I obtained **two standard GACR grants and collaborative grant from European Regional Development Fund** - Program Interreg V-A Austria-Czech Republic (see list of grants for more details). I established a number of collaborations with theoretical and experimental groups (for details see CV). Currently**, I supervise 3 PhD, 3 Master, and 2 undergraduate students**. 2 Master and one bachelor students finished their theses under my supervision. My teaching activities gradually increased and, currently, I lecture advanced courses in field of computer simulations as well as an obligatory course on physics of biopolymers for bachelor students. Due to my unique expertise I also lecture a specialized course at Charles University in Prague. **I became associate professor (habilitated) at Faculty of Mathematics and Physics, Charles University in Prague in 2016.** At CEITEC I have been publishing papers in renowned journals including **Angewandte Chemie International Edition (IF= 10.777) and Journal of the American Chemical Society (JACS, IF:11.444**).

Education:

09/05 - 06/09 **Ph.D.** thesis: ***"Molecular simulations of surfaces of aqueous solutions"*** with **Pavel Jungwirth** at Faculty of Science, Charles University in Prague, Czech Republic

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09/99 – 06/04 Scholarship for the 50 best students in each year (about 10% of all students)

Outline of research plan for the next 3 years

Protein-protein and protein-membrane interactions are key players in cellular signaling, transport, and host defense. Alterations of these interactions are related to a number of diseases ranging from cancer to Alzheimer's disease. However, the dependence of the interaction between a particular protein sequence + structure and lipid composition remains elusive.[1] We have demonstrated the influence of membrane composition on the aggregation of amyloid peptides in a pilot study considering three types of lipids.[2] **We plan to further investigate amyloid and other protein-membrane and protein-protein interactions using computer simulations (from the coarse-grained to all-atom level) with a focus on specific effects of lipids** – for details, see projects below. The information obtained, including our recent results[2], can be used for diagnosing the risks of diseases, developing new therapeutic peptides (antimicrobial peptides, sensors, target specific drug carriers), and suggesting new treatment strategies (including lipid diet and altering lipid metabolism).[3]

Our multi-scale simulation approach and expertise in lipid membranes and proteins is our major advantage unique in CEITEC MU and rare worldwide. We can provide complementary data to experiments and reveal the underlying molecular mechanism with all-atom detail. This has already proved to be useful and **we have already established several local as well as external collaborations (see CV). Within CEITEC, we have collaborations with the group of Dr. Pavel Plevka and the Cryo-electron Microscopy and Tomography core facility**, which has been granted financial support from the international Interreg grant (2016-2019) to investigate protein-protein interactions and the dynamics of viruses. With the support of a new standard GACR grant (2017-2019) we will establish protein-membrane interaction experiments in CEITEC MU, in which we expect to collaborate with the Biomolecular Interactions and Crystallization core facility and Imaging core facility, in order to determine the binding strengths of proteins to membranes.

I have already established a research team consisting of three PhD students, three Master's students, and two undergraduate students. We aim to meet the systemization requirements of CEITEC MU by 2019, for which **I have already obtained both independent and collaborative funding** (GACR and Interreg), which allowed me to have opening for two additional PhD students). In addition, I have a postdoc SoMoPro application under evaluation. In the more distant future (4 years), I plan to stabilize the group by applying for long-term funding such as the ERC consolidator grant. My previous ERC starting application is highly encouraging by being rated B. The main criticism was lack of experimental experience, which am I addressing by establishing a wet lab for lipid experiments (supported from the newly awarded standard GACR grant). In addition, I am also participating in OP VVV and GAMU grant applications that are currently under evaluation.

Projects:

1. **Abeta peptides** – (Daniel Jaroň, Peter Pajtinka) Alzheimer's Disease (AD) is the most common form of dementia in the elderly. Currently, 1 in 8 people above the age of 65 suffer from this disorder, and it is expected that there will be 115 million people affected globally by 2050, with treatment costing over $2,000 billion/year.[4] Amyloid-β (Aβ) peptide has been identified as a clinical hallmark in the disease's development and progression. Its oligomers are recognized as the most toxic species, which act by disrupting neuronal membranes. However, the relation between the membrane composition and its effect on Aβ oligomerisation remains unclear. **We will determine**

[1] McMahon, H. T.; Boucrot, E.: J. Cell Sci. 2015, 128, 1065–1070. Hubner, C. A.; et al.: Brain 2014, 137, 3109–3121.
[2] Amaro, M.; et al. Vacha, R.; Hof, M.: Angew. Chem. Int. Edit. 2016, 55,9411; VIP Paper.
[3] Berglund, L.; et al.: J. Clin. Endocrinol. Metab. 2012,97(9), 2969–2989.
[4] Mullane, K.; Williams, M. Biochem. Pharmacol. 2013, 85, 289.

how gangliosides influence Aβ behavior and we will also characterize the molecular mechanism by which they prevent or accelerate Aβ oligomerisation.[5] We have recently shown how Aβ oligomerisation can be prevented by physiological concentrations of ganglioside GM1.[6] Using state-of-the-art molecular dynamics simulations with advanced sampling techniques (e.g. Hamiltonian Replica Exchange), coupled with single-molecule fluorescence microscopy and spectroscopy experiments, we will investigate other neuronal gangliosides in order to provide an atomic-level understanding of their interaction with Aβ peptides, which could be used in clinical applications.

2. **Antimicrobial peptides** – (Ivo Kabelka, Alžběta Türková) More than 0.7 million deaths/year are caused by drug-resistant bacteria and that number is estimated to grow to 10 million in 2050.[7] This is why growing microbial resistance and the slower development of new antibiotics was identified as a serious threat to global public health by the World Health Organization. Antimicrobial peptides are one of the candidates for new antibacterial treatments. With the right properties, peptides can kill bacteria, viruses, or even cancer cells by disrupting their membranes. Indeed, peptides are part of the antimicrobial immune system of many organisms, but they can also be toxic.[8] **By means of computer simulations we will systematically investigate the complex interplay between helical peptides and the most common lipids from bacterial and human membranes in order to identify the effect of length, flexibility, and distribution of hydrophobic residues that lead to peptide translocation and pore formation at various membranes.** The molecular understanding obtained will be used for the rational design of new antimicrobial peptides.

3. **Signaling proteins** – (Miroslav Jurásek, Tereza Gerguri, Ľubomíra Valová) Proteins involved in signaling pathways are vital for cells, and their malfunction is typically related to cancer or other diseases. We will focus on proteins that are associated with membranes, which are crucial not only for the protein's proper functioning but also for correct distribution/positioning within the cell. Currently, there are no rules for how to recognize which membrane a protein will localize to based on its sequence, post-translational modifications, and structure.[9] We will start with computer simulations of three specific proteins: [1] Dishevelled protein (DVL) from the Wnt signaling pathway; [2] protein kinase D; and [3] DivIVA protein binding to negatively curved membranes. Our long-term goal is **to decipher the protein-membrane relationship and provide rules and tools that will enable determination of a protein's preference for a membrane with a specific shape and composition**. This will provide an insight into the organization of proteins in cells and bring useful information for the design of targeted protein drug carriers and sensors.

4. **Virus Proteins** – (Lukáš Sukeník, Miroslav Jurásek, Daniel Jaroň) Viruses are ubiquitous deadly machines that cause a wide range of diseases from the common cold and flu to lethal HIV, Ebola, or SARS. Due to recent progress in electron microscopy, an increasing number of virus structures are being determined and can be further studied in order to identify the molecular mechanism of infection and find ways to prevent it. **We will investigate the interactions and dynamics of proteins from viruses (Bacteriophage phi812 and SBPV) with the main focus on structural changes related to infection and virus interactions with membranes.** This will be conducted in close collaboration with experiments including high-speed atomic force microscopy and cryo-electron microscopy. This combination will lead to the unprecedented temporal and spatial resolution of the underlying molecular refolding, a knowledge useful for biotechnology and development of new treatments.

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[5] Ledeen, R. Trends Neurosci. 1985, 8, 169. Kreutz, F.; et al. Neurochem. Int. 2011, 59, 648.
[6] Amaro, M.; et al. Vacha, R.; Hof, M.: Angew. Chem. Int. Edit. 2016, 55, 9411; VIP Paper.
[7] WHO: Review on Antimicrobial Resistance by Jim O'Neill, 2014.
[8] Zasloff, M. Nature 2002, 415, 389–95. Freire, J. M. et al. J. Pept. Sci. 2015, 21, 178–185.
[9] Uhlén M et al, Science 2015, 347, 6220; www.proteinatlas.org.

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