PERSONAL INFORMATION

Family name, First name: **Vacha, Robert**
Date of birth: 29th December 1980
ResearcherID, ORCID: M-3809-2019, 0000-0001-7610-658X
URL for web site: http://vacha.ceitec.cz/
H-index, articles, citations: 36, 83, 4500

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

POSITIONS:

05/23 – **Group leader and Professor,** CEITEC (Central European Institute of Technology) and Faculty of Science at Masaryk University, Brno (Czech Republic)

07/17 – 5/23 **Junior group leader,** CEITEC (Central European Institute of Technology) and Faculty of Science at Masaryk University, Brno (Czech Republic)

04/16 – 06/17 **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 **Short 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:

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

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

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

2006 – 2008 **Assistant** teacher of *Classical molecular dynamics* at Faculty of Mathematics and Physics, Charles University in Prague

PhD opponent/examiner at ETH Zurich, Lund University, Imperial College London, Tampere University of Technology, Charles University in Prague, University of Chemistry and Technology Prague, and Palacky University Olomouc

GRANTS:

2025 – 2026 European Research Council, Proof of Concept Grant (**ERC**) – PI, Fighting Resistant Bacteria with Antimicrobial Peptides, 1 year (150 000 EUR)

2025 – 2027 Czech Science Foundation grant (**GACR**) – PI, How lipid asymmetry influences membrane protein function, 3 years (210 000 EUR)

2025 – 2025 Technology Agency of the Czech Republic (**TACR**) – PI, In vivo efficacy of peptides against bacterial infection in mice, 1 year (85 000 EUR)

2022 – 2025 National Institute of Virology and Bacteriology (**NIVB**) – member, 3,5 years (1 600 000 EUR)

2022 – 2026 European Research Council, Consolidator Grant (**ERC**) – PI, Peptide Killers, 5 years (2 300 000 EUR)

2020 – 2025 Ministry of Education Youth and Sports o Czech Republic (**ERC CZ**) – PI, Peptide Killers, 5 years (2 500 000 EUR)

2020 – 2022 Czech Science Foundation grant (**GACR**) – PI, Protein Affinity and Selectivity to Cellular Membranes, 3 years (320 000 EUR)

2018 – 2019 Technology Agency of the Czech Republic (**TACR**) – PI, Toxicity and Activity of Antimicrobial Peptides, 1 year (31 000 EUR)

2017 – 2019 Czech Science Foundation grant (**GACR**) – PI, Amphiphilic Peptides at Phospholipid Membranes, 3 years (180 000 EUR)

2017 – 2019 Grant Agency of Masaryk University (**GAMU**) – co-PI, Computational chemistry for Wnt signaling pathway, 3 years (190 000 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)

INSTITUIONAL RESPONSIBILITIES:

07/23 – Scientific coordinator of National Institute of Virology and Bacteriology

03/23 – Scientific board member of ICS MU

06/22 – Coordination board of National Institute of Virology and Bacteriology

11/21 – Scientific board member of CEITEC MU

04/23 – 03/25 Chair of Czech Science Foundation biophysics panel

04/21 – 03/23 Vice-chair of Czech Science Foundation biophysics panel

01/21 – Member of User Board of e-INFRA

07/20 – Member of Information Technologies Board of the Masaryk University

07/19 – Head of CEITEC IT committee

INVITED LECTURES (selected):

2024 CECAM Flagship workshop - Physics of mesoscale liquid condensates, Lyiiang, China

2024 CECAM workshop - Exploring bio-inspired systems: a synergy between multiscale experimental and computational approaches, Vienna, Austria
2024 Biophysics Austria Conference 2024, Salzburg, Austria
2024 CECAM Flagship workshop - Peptides in Biology and Materials: Bridging Simulation and Experimental Data, Florence, Italy
2022 Invited seminars at Imperial college, UK; International Institute of Molecular and Cell Biology in Warsaw, Poland; Heyrovsky Institute AVCR, Charles University, and University of Ostrava, Czech Republic
2021 EJTEMM 2021 – Graz, Austria
2018 43rd FEBS Congress Prague, Czech Republic
2018 CECAM workshop - Nano-structured soft matter: a synergy of approaches to amphiphilic and block copolymer systems, Lincoln, United Kingdom
2018 CECAM workshop - Frontiers in Computational Biophysics, Lugano, Switzerland
2017 CECAM workshop - The future of biomembrane simulations: hidden pitfalls and future challenges, Lyon, France
2017 Joint Meeting of Czech and German Biophysicists, Hünfeld, Germany
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

ALUMNI:
3 postdocs, 5 PhD students, 11 MSc students, 8 Bc students

AWARDS:

2024 MUNI Scientist, CEITEC MU Award
2024 elected member of Czech Learned Society
2022 Award of rector of Masaryk university, Bronze medal of Masaryk University, CEITEC MU award
2021 MUNI Scientist
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)

MAJOR RESEARCH COLLABORATIONS:

Karl Lohner and Georg Pabst– University of Graz, Austria – SAXS, SANS, leakage assays, antimicrobial peptide activity (5 joint papers and 1 in preparation)
Pavel Plevka – Masaryk University, Czech Republic – CryoEM of viruses and their interactions (4 joint papers and 1 paper in preparation)
Mikael Lund – Lund University, Sweden – Development of new protein models and Monte Carlo methods (8 joint papers)
Martin Hof – Academy of Sciences, Czech Rep. – Fluorescence measurements on phospholipid membranes and proteins (6 joint papers)

PUBLICATIONS:

I have published 83 peer-reviewed articles, one book chapter and three editorial comments in major international journals that have attracted more than 4500 citations (excluding self-citations according to ISI Web of Science in Feb 2025), yielding an H-index of 36. These publications include Nature Communication, PNAS, Nano letters, ACS Nano, JACS, Angewandte Chemie, eLife, Science Advances, and Accounts of Chemical Research.

Publication record of the PI according to the ISI Web of Science in January 2025:

83. Savenko, M.; **Vácha, R.**; Ramseyer, C.; Rivel, T.;: Role of Divalent Ions in Membrane Models of Polymyxin-Sensitive and Resistant Gram-Negative Bacteria. *Journal of Chemical Information and Modeling* 2025, 65, 3, 1476–1491, IF=5.7

82. Rivel, T.; Biriukov, D.; Kabelka, I.; **Vácha, R.**: Free Energy of Membrane Pore Formation and Stability from Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling* 2025, 65, 2, 908–920, IF=5.7

81. Hazrati, M.K.; Sukeník, L.; **Vácha, R.**: Split Membrane: A New Model to Accelerate All-Atom MD Simulation of Phospholipid Bilayers. *Journal of Chemical Information and Modeling* 2025, 65, 2, 845–856, IF=5.7

79. Bartoš, L.; Lund, M.; **Vácha, R**.: Enhanced Diffusion through Multivalency. *Soft Matter* 2025, 21, 179-185, IF=2.9

78. Linhartova, K.; Falginella, F.L.; Matl, M.; Šebesta, M.; **Vácha, R**.; Štefl, R.: Sequence and structural determinants of RNAPII CTD phase-separation and phosphorylation by CDK7. *Nature Communications* 2024, 15, 9163, IF=14.7

77. Hazrati, M.K.; **Vácha, R.**: Membrane Adsorption Enhances Translocation of Antimicrobial Peptide Buforin 2. *The Journal of Physical Chemistry B* 2024, 128, 35, 8469–847, IF=2.8

76. Deb, R.; Torres, M.D.T.; Boudný, M.; Koběrská, M.; Cappiello, F.; Popper, M.; Dvořáková Bendová, K.; Drabinová, M.; Hanáčková, A.; Jeannot, K.; Petřík, M.; Mangoni, M.L.; Balíková Novotná, G.; Mráz, M.; de la Fuente-Nunez, C.; **Vácha, R.**: Computational Design of Pore-Forming Peptides with Potent Antimicrobial and Anticancer Activities. *Journal of Medicinal Chemistry* 2024, 67, 16, 14040–14061, IF=6.8

75. Blasco S.; Sukeník, L.; **Vácha, R.**: Nanoparticle induced fusion of lipid membranes. *Nanoscale* 2024, 16, 10221-10229, IF=8.3

74. Bartoš, L.; Drabinová, M.; **Vácha, R.**: Optimizing properties of translocation-enhancing transmembrane proteins. *Biophysical Journal* 2024, 123, 1–13, IF=3.7

73. Morton, W.; **Vácha, R.**; Angioletti-Uberti, S.: Valency of Ligand–Receptor Binding from Pair Potentials. *Journal of Chemical Theory and Computation* 2024, 20, 7, 2901–2907, IF=5.5

72. Bartoš, L.; **Vácha, R.**: Peptide translocation across asymmetric phospholipid membranes. *Biophysical Journal* 2024, 123, 1-10, IF=3.7

71. Bartoš, L.; Menon, A.K.; **Vácha, R.**: Insertases Scramble Lipids: Molecular Simulations of MTCH2. *Structure* 2024, 32, 4, 505-510, IF=5.7

70. Bartoš, L.; **Vácha, R**.: Peptide translocation across asymmetric phospholipid membranes. *Biophysical Journal* 2024, 123, 1-10, IF=3.4

69. Pajtinka, P.; **Vácha, R.**: Amphipathic Helices Can Sense Both Positive and Negative Curvatures of Lipid Membranes. *The Journal of Physical Chemistry Letters* 2024, 15, 175−179, IF=5.7

68. Jahn, H.; Bartoš, L.; Dearden, G.I.; Dittman, J.S.; Holthuis, J.C.M.; **Vácha, R.**; Menon, A.K.: Phospholipids are imported into mitochondria by VDAC, a dimeric beta barrel scramblase. *Nature Communications* 2023, 14, 8115, IF=16.6

67. Semeraro, E.F.; Pajtinka, P.; Marx, L.; Kabelka, I.; Leber, R.; Lohner, K.; **Vácha, R**.; Pabst, G.: Magainin 2 and PGLa in Bacterial Membrane Mimics IV: Membrane Curvature and Partitioning. *Biophysical Journal* 2022, 121, 1-13, IF=4.033

66. Falginella, F.L.; Kravec, M.; Drabinová, M.; Paclíková, P., Bryja, V.; **Vácha, R**.: Binding of DEP domain to phospholipid membranes: More than just electrostatics**.** *BBA - Biomembranes* 2022, 1864 (10), 183983, IF=3.747

65. Khirsariya, P.; Pospíšil, P.; Maier, L.; Boudný, M.; Babáš, M.; Kroutil, O.; Mráz, M.; **Vácha, R.**; Paruch, K.: Synthesis and Profiling of Highly Selective Inhibitors of Methyltransferase DOT1L Based on Carbocyclic C-Nucleosides. *Journal of Medicinal Chemistry* 2022, i2022, 65, 7, 5701–5723, IF= 7.446

64. Kabelka, I.; Georgiev, V.; Marx, L.; Pajtinka, P.; Lohner, K.; Pabst, G.; Dimova, R.; **Vácha, R**.: Magainin 2 and PGLa in Bacterial Membrane Mimics III: Membrane Fusion and Disruption. *Biophysical Journal* 2022, 121 (5), 852-861, IF=4.033

63. Sukeník, L.; Mukhamedova, L.; Michaela Procházková, M.; Karel Škubník, K.; Pavel Plevka, P.; **Vácha, R.**: Cargo Release from Nonenveloped Viruses and Virus-like Nanoparticles: Capsid Rupture or Pore Formation. *ACS Nano* 2021, 15, 12, 19233–19243, IF= 15.881

62. Sarmento, M.J.; Owen, M.C.; Ricardo, J.C.; Chmelová, B.; Davidović, D.; Mikhalyov, I.; Gretskaya, N.; Hof, M.; Amaro, M.; **Vácha, R.**; Šachl, R.: The impact of the glycan headgroup on the nanoscopic segregation of gangliosides. *Biophysical Journal* 2021, 120 (24), 5530-5543, IF=3.665

61. Bartoš, L.; Kabelka, I.; **Vácha, R.**: Enhanced translocation of amphiphilic peptides across membranes by transmembrane proteins. *Biophysical Journal* 2021, 120 (11), 2296-2305, IF=3.665

60. Kabelka, I.; **Vácha, R**.: Advances in Molecular Understanding of α-helical Membrane-Active Peptides**.** *Accounts of Chemical Research* 2021, 54 (9), 2196–2204, IF=21.661

59. Procházková, M., Füzik, T., Grybchuk, D., Falginella, F., Podešvová, L., Yurchenko, V., **Vácha, R.**, Plevka, P. Capsid structure of Leishmania RNA virus 1. *Journal of Virology* 2021, 95, e01957-20. IF=4.501

58. Jurásek, M.; Kumar, J.; Paclíková, P.; Kumari, A.; Tripsianes, K.; Bryja, V.; **Vácha, R.**: Phosphorylation-induced changes in the PDZ domain of Dishevelled 3. *Scientific Reports* 2021, 11, 1484, IF= 3.998

57. Kabelka, I.; Brožek, R**.; Vácha, R.**: Selecting Collective Variables and Free Energy Methods for Peptide Translocation Across Membranes. *Journal of Chemical Information and Modeling* 2021, 61, 2, 819–830, IF= 4.549

56. Škubník, K.; Sukeník, L.; Buchta, D.; Füzik, T.; Procházková, M.; Moravcová, J.; Šmerdová, L.; Přidal, A.; **Vácha, R.**; Plevka, P.: Capsid opening enables genome release of iflaviruses. *Science Advances* 2021, 7(1), eabd7130, IF= 13.116

55. Brožek, R.; Kabelka, I.; **Vácha, R.**: Effect of Helical Kink on Peptide Translocation across Phospholipid Membranes. *Journal of Physical Chemistry B* 2020,124, 28, 5940-5947, IF=2.857

54. Brázda, R.; Krejčíková, M.; Kasiliauskaite, A.; Šmiřáková, E.; Klumpler, T.; **Vácha, R.**; Kubíček, K.; Štefl, R.: Yeast Spt6 reads multiple phosphorylation patterns of RNA Polymerase II C-terminal domain in vitro. *Journal of Molecular Biology* 2020, 432(14), 4092-4107, IF=4.76

53. Tuerkova, A.; Kabelka, I.; Králová, T.; Sukeník, L.; Pokorná, Š.; Hof, M.; **Vácha, R.**: Effect of helical kink in antimicrobial peptides on membrane pore formation. *eLife* 2020, 9, e47946, IF=7.551

52. Jurásek, M.; Flärdh, K.; **Vácha, R.**: Effect of membrane composition on DivIVA-membrane interaction. BBA Biomembranes 2020, 1862, 8, 183144, IF=3.411

51. Kabelka, I.; Pachler, M.; Prévost, S.; Letofsky-Papst, I.; Lohner, K.; Pabst, G.; **Vácha, R.**: Magainin 2 and PGLa in Bacterial Membrane Mimics II: Membrane Fusion and Sponge Phase Formation. *Biophysical Journal* 2020, 118, 3, 612-623, IF=3.665

50. Pachler, M.; Kabelka, I.; Appavou, M.-S.; Lohner, K.; **Vácha, R.**; Pabst, G.: Magainin 2 and PGLa in Bacterial Membrane Mimics I: Peptide-Peptide and Lipid-Peptide Interactions. *Biophysical Journal* 2019, 117, 1858–1869, IF=3.665

49. Owen, M.C.; Karner, A.; Šachl, R.; Preiner, J.; Amaro, M.; **Vácha, R.**: Force Field Comparison of GM1 in a DOPC Bilayer Validated with AFM and FRET Experiments. *Journal of Physical Chemistry. B* 2019, 123, 35, 7504-7517, IF=2.923

48. Buchta, D.; Füzik, T.; Hrebík, D.; Levdansky, Y.; Sukeník, L.; Mukhamedova, L.; Moravcová, J.; **Vácha, R.**; Plevka, P.: Enterovirus particles expel capsid pentamers to enable genome release. *Nature Communication* 2019, 10, 1138, IF=12.353

47. Harnoš, J.; Alonso Cañizal, M.C.A.; Jurásek, M.; Kumar, J.; Holler, C.; Schambony, A.; Hanáková, K.; Bernatík, O.; Zdráhal, Z.; Gömöryová, K.; Gybeľ, T.; Radaszkiewicz, T.W.; Kravec, M.; Trantírek, L.; Ryneš, J.; Dave, Z.; Fernández-Llamazares, A.I.; **Vácha, R.**; Tripsianes, K.; Hoffmann, C.; Bryja, V.: Dishevelled-3 conformation dynamics analyzed by FRET-based biosensors reveals a key role of casein kinase 1. *Nature Communication* 2019, 10, 1804, IF=12.353

46. Kabelka, I.; **Vácha, R.**: Optimal Hydrophobicity and Reorientation of Amphiphilic Peptides Translocating Through Membrane. *Biophysical Journal* **2018**, 115 (6), 1045-1054, IF=3.632

45. Leber, R.; Pachler, M.; Kabelka, I.; Svoboda, I.; Koller, D.; **Vácha, R**.; Lohner, K.; Pabst, G.: Synergism of Antimicrobial Frog Peptides Couples to Membrane Intrinsic Curvature Strain. *Biophysical Journal* 2018, 114 (8), 1945-1954, IF=3.632

44. Tesei, G.; Hellstrand, E.; Sanagavarapu, K.; Linse, S.; Sparr, E.; **Vácha, R.**; Lund, M.: Aggregate Size Dependence of Amyloid Adsorption onto Charged Interfaces. *Langmuir* **2018**, 34 (4), 1266–1273, IF=4.384

43. Schubertová, V.; Martinez-Veracoechea, F.J.; **Vácha, R**.: Design of Multivalent Inhibitors for Preventing Cellular Uptake. *Scientific Reports* **2017**, 7, 11689, IF= 4.259

42. Jurásek, M.; **Vácha, R.**: Self-assembled clusters of patchy rod-like molecules. *Soft Matter* **2017**, 13, 7492 – 7497, IF=3.889

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

40. 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

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

38. **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

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

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

35. 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

34. 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

33. **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

32. 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

31. **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

30. 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

29. 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

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

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