

PERSONAL INFORMATION

Family name, First name: **Vacha, Robert**
Date of birth: 29th December 1980
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URL for web site: <http://vacha.ceitec.cz/>
H-index, articles, citations: 37, 86, >5000

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, University of Lyon, Charles University in Prague, University of Chemistry and Technology Prague, and Palacky University Olomouc

GRANTS:

2026 – 2028 Czech Science Foundation grant (**GACR**) – PI, Design Principles of Fusogenic Proteins for Lipid Vesicles, 3 years (430 000 EUR)

2025 – 2027 INTER-COST MŠMT– PI, Peptides controlling membrane curvature, 2 years (192 000 EUR)

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 of 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)

INSTITUTIONAL 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):

- 2026 Peptides in biology and materials: bridging simulation and experimental data, Sofia, Bulgaria
- 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, 9 PhD students, 12 MSc students, 8 Bc students

AWARDS:

- 2025 MUNI Scientist and Vice-rector's award, Masaryk University
- 2025 Frantisek Behounek award from the Ministry of Education, Youth and Sports of the Czech Republic
- 2025 Rector's Award for significant creative achievement, Masaryk University
- 2024 MUNI Scientist and CEITEC MU Award, Masaryk University
- 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, Masaryk University
- 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:

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 86 peer-reviewed articles, one book chapter and three editorial comments in major international journals that have attracted more than 5000 citations (excluding self-citations according to ISI Web of Science in Feb 2026), yielding an H-index of 37. 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 April 2026:

86. Blasco, S.; Spearing, E.; Drabinová, M.; Rašková, V.; **Vácha, R.**: Implicit membrane for helical peptide selectivity toward bacterial membranes. *Biophysical Journal* 2026, in press

85. Sushmita, P.; Pajtinka, P.; Javanainen, M.; **Vácha, R.**: Helical sensors of membrane saturation: Changes in orientation and curvature preference. *Biophysical Journal* 2025, 124, 23, 4087-4095, IF=3.1

84. Kroutil, O.; Bartoš, L.; Kabelka, I.; **Vácha, R.**: Martini 3 Limitations in Phospholipid Flip-Flop. *Journal of Chemical Theory and Computation* 2025, 21, 19, 9227–9233, IF=5.5

83. Yadav, A.K.; Jadhav, A.S.; Szczepanik, P.M.; Fagherazzi, K.; Kabelka, I.; **Vácha, R.**; Švenda, J.; Polášek-Sedláčková, H.: A biotin-HaloTag ligand enables efficient affinity capture of protein variants from live cells. *Journal of Cell Biology* 2025, 224 8, e202410025, IF=6.4

82. Bartoš, L.; Pajtinka, P.; **Vácha, R.**: gorder: Comprehensive tool for calculating lipid order parameters from molecular simulations. *SoftwareX* 2025, 31, 102254, IF=2.4

81. 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

80. 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

79. 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

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

77. 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
76. 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
75. Deb, R.; Torres, M.D.T.; Boudný, M.; Koběřská, 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
74. Blasco S.; Sukeník, L.; **Vácha, R.**: Nanoparticle induced fusion of lipid membranes. *Nanoscale* 2024, 16, 10221-10229, IF=8.3
73. Bartoš, L.; Drabinová, M.; **Vácha, R.**: Optimizing properties of translocation-enhancing transmembrane proteins. *Biophysical Journal* 2024, 123, 1–13, IF=3.7
72. 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
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.; Gretskeya, 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 flaviruses. *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.; Gybel, 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
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