Dr. Volodymyr Farafonov

curriculum vitae

➢ Personal data

Other names: Vladimir S. Farafonov
Date of birth: 10 November 1992
Nationality: Ukraine

➢ Contact information

Job address: Department of Physical Chemistry, School of Chemistry,
V. N. Karazin Kharkiv National University, 4 Svoboda sq., Kharkiv, 61022, Ukraine
Job phone: (057) 707 54 45
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Job e-mail: farafonov@karazin.ua

➢ Education

18.12.2018:	Ph.D. degree awarded for the thesis «Localization and hydration of organic dyes in surfactant micelles by molecular dynamics simulations» (specialty «Physical chemistry», code 02.00.04)
11.2014 – 03.2018:	Ph.D. student at the Department of Physical Chemistry, School of Chemistry, V.N. Karazin Kharkiv National University (KhNU)
09.2009 – 06.2014:	Undergraduate student at the School of Chemistry, KhNU

➢ Employment

01.2020 – *present*	Senior Research Fellow	Department of Physical Chemistry, KhNU
01.2018 – 01.2020	Research Fellow	*same place*
09.2019 – *present*	Assistant Professor	*same place*
04.2018 – 09.2019	Teacher	*same place*
05.2018 – *present*	Visiting Research Fellow	School of Engineering and Applied Science, Aston University, Birmingham, UK
10.2017 – 01.2018	Research Associate	*same place*
03.2017 – 05.2017	Engineer	Research Institute of Chemistry, KhNU
03.2016 – 06.2016	Junior Research Fellow	Department of Physical Chemistry, KhNU

➢ Research interests

— Investigation of micellar solutions with molecular dynamics
— Computer simulations of biomolecules, in particular, viruses
— Participation in development of multiscale molecular dynamics/fluctuating hydrodynamics method

➢ Honours and awards

— Winner of the district stage of the municipal competition «Young person of the year — 2020» in nomination «Scientific activity» (in Kharkiv city)
— Laureate of the Award of Supreme Council of Ukraine for young scientists in 2019 (as a member of a collective for the work „Complex ecological approach to design of novel functional materials for chemical analysis and technology")
— Associate member of the Royal Society of Chemistry from 2016 (membership number 620846)

➢ Publications

— h-index 8 (Scopus)
— 29 articles, including 19 Scopus-cited
— 23 conference papers, including 13 papers for international conferences

Selected articles in Scopus-cited journals:

1. **Farafonov, V. S.**, Stich, M., Nerukh, D. Reconstruction and validation of entire virus model with complete genome from mixed resolution cryo-EM density. *Faraday Discuss.* **2022**, DOI: 10.1039/D2FD00053A
2. Abdelhalim, A. O. E.; Sharoyko, V. V.; Ageev, S. V.; **Farafonov, V. S.**; Nerukh, D. A.; Postnov, V. N.; Petrov, A. V.; Semenov, K. N. Graphene Oxide of Extra High Oxidation: A Wafer for Loading Guest Molecules. *J. Phys. Chem. Lett.* **2021**, 12, 10015−10024, DOI: 10.1021/acs.jpclett.1c02766
3. Li, F.; Korotkin, I.; **Farafonov, V.**; Karabasov, S. Lateral migration of peptides in transversely sheared flows in water: An atomistic-scale-resolving simulation. *J. Mol. Liq.* **2021**, *337*, 116111, DOI: 10.1016/j.molliq.2021.116111
4. **Farafonov, V. S.**; Lebed, A. V., Mchedlov-Petrossyan, N. O. Computing pK_a Shifts Using Traditional Molecular Dynamics: Example of Acid–Base Indicator Dyes in Organized Solutions. *J. Chem. Theory Comput.* **2020**, *16* (9), 5852–5865, DOI: 10.1021/acs.jctc.0c00231
5. **Farafonov, V. S.**, Nerukh, D. MS2 bacteriophage capsid studied using all-atom molecular dynamics. *Int. Focus* **2019**, *9*, 20180081, DOI: 10.1098/rsfs.2018.0081
6. Tarasova, E.; **Farafonov, V.**; Taiji, M.; Nerukh, D. Details of charge distribution in stable viral capsid. *J. Mol. Liq.* **2018**, *265*, 585–591, DOI: 10.1016/j.molliq.2018.06.019
7. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrossyan, N. O. Character of localization and microenvironment of solvatochromic Reichardt's betaine dye in sodium *n*-dodecyl sulfate and cetyltrimethylammonium bromide micelles: molecular dynamics simulation study. *Langmuir* **2017**, *33*, 8342−8352, DOI: 10.1021/acs.langmuir.7b01737
8. **Farafonov, V. S.**; Lebed, A. V. Developing and validating a set of all-atom potential models for sodium dodecyl sulfate. *J. Chem. Theory Comput.* **2017**, *13*, 2742–2750, DOI: 10.1021/acs.jctc.7b00181
9. Tarasova, E.; **Farafonov, V.**; Khayat, R.; Okimoto, N.; Komatsu, T.; Taiji, M.; Nerukh, D. All-atom molecular dynamics simulations of entire virus capsid reveal the role of ion distribution in capsid's stability. *J. Phys. Chem. Lett.* **2017**, *8*, 779–784, DOI: 10.1021/acs.jpclett.6b02759
10. Tarasova, E.; Korotkin, I.; **Farafonov, V.**; Karabasov, S.; Nerukh, D. Complete virus capsid at all-atom resolution: Simulations using molecular dynamics and hybrid molecular dynamics/hydrodynamics methods reveal semipermeable membrane function. *J. Mol. Liq.* **2017**, *245* (Supplement C), 109–114, DOI: 10.1016/j.molliq.2017.06.124

11. Korotkin, I.; Nerukh, D.; Tarasova, E.; **Farafonov, V.**; Karabasov, S. Two-phase flow analogy as an effective boundary condition for modelling liquids at atomistic resolution. *J. Comput. Sci.* **2016**, *17* (part 2), 446–456, DOI: 10.1016/j.jocs.2016.03.012

Other articles in Scopus-cited journals:

1. Maximova, E.; Postnikov, E. B.; Lavrova, A. I.; **Farafonov, V.**; Nerukh, D. Protein-Ligand Dissociation Rate Constant from All-Atom Simulation. *J. Phys. Chem. Lett.* **2021**, 12, 10631–10636, DOI: 10.1021/acs.jpclett.1c02952
2. Sharoyko, V.; Iamalova, N. R.; Ageev, S. V.; Meshcheriakov, A. A.; Iurev, G. O.; Petrov, A. V.; Nerukh, D. A.; **Farafonov, V. S.**; Vasina, L. V.; Penkova, A. V.; Semenov, K. N. *In Vitro* and *In Silico* Investigation of Water-Soluble Fullerenol $C_{60}(OH)_{24}$: Bioactivity and Biocompatibility. *J. Phys. Chem. B* **2021**, *125*, 9197–9212, DOI: 10.1021/acs.jpcb.1c03332
3. Wu, Y.; Okesola, B. O.; Xu, J.; Korotkin, I.; Berardo, A.; Corridori, I.; di Brocchetti, F. L. P.; Kanczler, J.; Feng, J.; Li, W.; Shi, Y.; **Farafonov, V.**; Wang, Y.; Thompson, R. F.; Titirici, M.-M.; Nerukh, D.; Karabasov, S.; Oreffo, R. O. C.; Rodriguez-Cabello, J. C.; Vozzi, G.; Azevedo, H. S.; Pugno, N. M.; Wang, W.; Mata, A. Disordered protein-graphene oxide co-assembly and supramolecular biofabrication of functional fluidic devices. *Nat. Commun.*, **2020**, *11*, 1182. DOI: 10.1038/s41467-020-14716-z
4. Vus, K.; Tarabara, U.; Balklava, Z.; Nerukh, D.; Stich, M.; Laguta, A.; Vodolazkaya, N.; Mchedlov-Petrossyan, N. O.; **Farafonov, V.**; Kriklya, N.; Gorbenko, G.; Trusova, V.; Zhytniakivska, O.; Kurutose, A.; Gadjev, N.; Deligeorgiev, T. Association of novel monomethine cyanine dyes with bacteriophage MS2: A fluorescence study. *J. Mol. Liq.* **2020**, *302*, 112569. DOI: 10.1016/j.molliq.2020.112569
5. Mchedlov-Petrossyan, N. O.; **Farafonov, V. S.**; Cheipesh, T. A.; Shekhovtsov, S. V.; Nerukh, D. A.; Lebed, A. V. In search of an optimal acid-base indicator for examining surfactant micelles: Spectrophotometric studies and molecular dynamics simulations. *Colloids Surf., A* **2019**, *565*, 97–107, DOI: 10.1016/j.colsurfa.2018.12.048
6. Mchedlov-Petrossyan, N. O.; **Farafonov, V. S.**; Lebed, A. V. Examining surfactant micelles via acid-base indicators: Revisiting the pioneering Hartley-Roe 1940 study by molecular dynamics modeling. *J. Mol. Liq.* **2018**, *264*, 683–690, DOI: 10.1016/j.molliq.2018.05.076
7. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrossyan, N. O. Solvatochromic betaine dyes of different hydrophobicity in ionic surfactant micelles: Molecular dynamics modeling of location character. *Colloids Surf., A* **2018**, *538*, 583–592, DOI: 10.1016/j.colsurfa.2017.11.046
8. Korotkin, I.; Karabasov, S.; Nerukh, D.; Markesteijn, A.; Scukins, A.; **Farafonov, V.**; Pavlov, E. A hybrid molecular dynamics/fluctuating hydrodynamics method for modelling liquids at multiple scales in space and time. *J. Chem. Phys.* **2015**, *143*, 014110, DOI: 10.1063/1.4923011

Articles in local journals:

1. **Farafonov, V. S.**; Lebed, A. V., Mchedlov-Petrossyan, N. O. Continuum electrostatics investigation of ionic micelles using atomistic models. *Ukr. Chem. J.* **2021**. 6, 87, 55–69, DOI: 10.33609/2708-129X.87.06.2021.55-69
2. **Farafonov, V. S.**; Lebed, A. V. Nitroxyl spin probe in ionic micelles: A molecular dynamics study. *Kharkov Univ. Bull., Chem. Ser.* **2020**, *34*, 57–64, DOI: 10.26565/2220-637X-2020-34-02
3. Tkachenko, V. V.; **Farafonov, V. S.**; Tokarev, V. V.; Tkachenko, I. G. Study of the effectiveness of various cannabinoid receptor 1 (CB1) agonists using molecular docking and molecular dynamics modeling. *Fr.-Ukr. J. Chem.* **2020**, *8* (1), 76–87. DOI: 10.17721/fujcV8I1P76-87

4. **Farafonov, V. S.**; Lebed, A. V.; Khimenko, N. L.; Mchedlov-Petrossyan, N. O. Molecular dynamics study of an acid-base indicator dye in Triton X-100 non-ionic micelles. *Voprosy Khimii i Khimicheskoi Tekhnologii* **2020**, *1*, 97–103. DOI: 10.32434/0321-4095-2020-128-1-97-103
5. Tarasova, E., **Farafonov, V.**, Nerukh, D. Molecular dynamics study of the role of ions in maintaining virus capsid stability. *Ensemble* **2019**, *21* (1), 50–54. DOI: 10.11436/mssj.21.50
6. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrossyan, N. O. An MD simulation study of Reichardt's betaines in surfactant micelles: unlike orientation and solvation of cationic, zwitterionic, and anionic dye species within the pseudophase. *Kharkov Univ. Bull., Chem. Ser.* **2018**, *30*, 27–35, DOI: 10.26565/2220-637X-2018-30-03
7. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrossyan, N. O. Examining solvatochromic Reichardt's dye in cationic micelles of different size via molecular dynamics. *Voprosy Khimii i Khimicheskoi Tekhnologii* **2018**, *5*, 62–68. http://vhht.dp.ua/wp-content/uploads/pdf/2018/5/Farafonov.pdf
8. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrossyan, N. O. Solvatochromic Reichardt's dye in micelles of sodium cetyl sulfate: MD modeling of location character and hydration. *Kharkov Univ. Bull., Chem. Ser.* **2017**, *28*, 5–11, DOI: 10.26565/2220-637X-2017-28-01
9. **Farafonov, V. S.**; Lebed, A. V. Molecular dynamics simulation study of cetylpyridinum chloride and cetyltrimethylammonium bromide micelles. *Kharkov University Bull., Chem. Ser.* **2016**, *27*, 25–30, DOI: 10.26565/2220-637X-2017-27-03
10. **Farafonov, V. S.**; Lebed, A. V. Molecular dynamics study of tetrapropylammonium ion localization in micellar solution of sodium dodecyl sulfate (in Russian). *Kharkov University Bull., Chem. Ser.* **2016**, *26*, 73–79, DOI: 10.26565/2220-637X-2017-26-08

Selected conference papers:

1. **Farafonov, V.S.**; Bakumenko, M., Yanushevskyi, A.; Bardik, V.; Pozhilenkov, A.; Kalachev, A.; Vaysfeld, N.; Stich, M.; Nerukh, D. All-atom MD of entire virus with genome in solution at physiological conditions. WATOC 2020, 12th Triennial Congress of the World Association of Theoretical and Computational Chemists, Vancouver, Canada, **2022**.
2. **Farafonov, V. S.**; Vodolazkaya, N.; Nikolskaya, M.; Laguta, A.; Balklava, Z.; Stich, M.; Mchedlov-Petrossyan, N.; Dmitry Nerukh, D. All-atom structure and dynamics of entire virus with genome in solution at physiological conditions. Faraday joint interest group conference (online), **2021**.
3. Vodolazkaya, N.; Nikolskaya, M.; Laguta, A.; **Farafonov, V.**; Balklava, Z.; Stich, M.; Mchedlov-Petrossyan, N.; Nerukh, D. Experimentally measured hydrophobicity and charge distribution on MS2 virus surface. Joint EMLG/JMLG Annual Meeting, 8-13 September 2019, Kutna Hora, Czech Republik, **2019**.
4. **Farafonov, V. S.**; Mchedlov-Petrossyan, N. O.; Lebed, A. V. Locus and local environment of two dyes in surfactant micelles from molecular dynamics simulations. Physics of Liquid Matter: Modern Problems: 8th International conference: Abstracts, 18-22 May 2018, Kyiv, Ukraine, **2018**.
5. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrossyan, N. O. Molecular dynamics study of locus of the standard Reichardt's indicator in ionic micelles. IXth International chemistry conference "Kyiv-Toulouse" dedicated to the 100th anniversary of Fedir Babichev: Materials of reports and performances, 4-9 June 2017, Kyiv, Ukraine**, 2017**.
6. Nerukh, D.; Karabasov S.; Tarasova, E.; Korotkin, I.; **Farafonov, V.**; Plyusnov, D.; Vaysfeld, N. Hybrid Molecular Dynamics - hydrodynamics modelling of liquidsolutions: whole virus at atomistic resolution. Joint EMLG/JMLG Annual Meeting, 10-14 September 2017, Vienna, Austria, **2017**.

7. **Farafonov, V. S.**; Nerukh, D. A.; Tarasova, E. A. Microscopic conditions in a virus capsid at molecular level. Physics for Life Sciences: I Russian conference, 12-16 September 2016, Saint Petersburg, Russia, **2016**.
8. Karabasov, S.; Korotkin, I.; Nerukh, D.; Tarasova, E.; **Farafonov, V.**; Markesteijn, A. Hybrid modelling based on two-phase flow analogy: advances and challenges. Hybrid Simulation Methods in Fluid Dynamics: Models, Software and Applications, Munich, Germany, **2015**.
9. Nerukh, D.; Karabasov, S.; Scukins, A.; Pavlov, E.; Korotkin, I.; **Farafonov, V.**; Taiji, M. Hybrid molecular dynamics–hydrodynamics framework for modelling liquid molecular systems: EMLG - JMLG annual meeting, 7-12 September 2014, Rome, Italy, **2014**.
10. **Farafonov, V. S.**; Lebed, A. V. Using molecular dynamics simulation for interpretation of Raman spectra of acetonitrile solution of sodium iodide. Karazin Chemistry Readings – 2014: VI All-Ukrainian scientific conference, 22-24 April 2014, Kharkiv, Ukraine, **2014**.

➢ Computer skills

Operating systems: advanced knowledge of Microsoft Windows; experience of Linux (including compilation and installation of software)
Desktop software: advanced knowledge of Microsoft Office, graphics editors
Scientific software: advanced knowledge of GROMACS, VMD, Origin; experience of GAMESS/FireFly, Gaussian, APBS, AIMPack, MathCAD.
Programming languages: advanced knowledge of C, Pascal/Delphi, AWK, Bash; experience of C#, TCL.

➢ Language skills

Ukrainian, Russian (native languages), English (level B2)

➢ Referees

Head of Department: Prof. Nikolay Mchedlov-Petrossyan
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Ph.D. co-supervisor: Dr. Dmitry Nerukh
Department of Mathematics, Aston University, Aston Triangle, Birmingham, B4 7ET, UK
Phone: +44 (0) 121 204 3533, e-mail: d.nerukh@aston.ac.uk

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