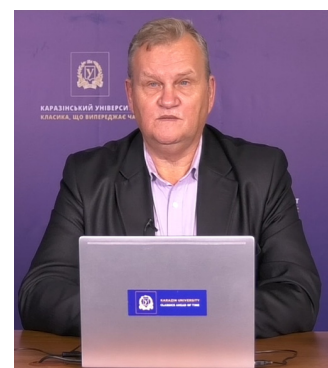


CURRICULUM VITAE

1. Family name: Lebed
First name: Alexander
Middle name: Valentinovich

2. Present position
Docent (Associate Professor),
Physical Chemistry Department,
V.N. Karazin Kharkiv National University
address
Svoboda sq., 4, Kharkiv - 22, 61022, UKRAINE
Tel: +38 (057) 7075445
E-mail: alebed@karazin.ua



3. Personal data
Title: Doctor
Date and place of birth: November 29, 1960; Kharkiv, UKRAINE
Nationality: Ukrainian
Marital status: married, two children

Period (from/to)	Name of institution	Position	Main subjects studied
09/1977-07/1982	Kharkiv State University	student	chemistry, physics, mathematics, English

5. Qualification
Master degree (in Chemistry) Kharkiv State University, 1982
PhD (Candidate of Science) Kharkiv State University, 1995

6. Employment
Period (from/to) Position Employer and place of work
11/2000 - till now Docent (Associate Professor) Physical Chemistry Department, KhNatUni
09/2000 - 10/2000 Docent (Associate Professor) Inorganic Chemistry Department, KhNatUni
06/1995 - 08/2000 Scientific researcher Inorganic Chemistry Department, KhNatUni
03/1992 - 06/1995 Junior researcher Inorganic Chemistry Department, KhStUni
11/1982 - 03/1992 Junior researcher Institute of Chemistry, KhStUni

7. Subjects read at the Kharkiv National University

- Physical Chemistry
- Colloidal Chemistry
- Medical Chemistry
- Theoretical Methods for Solvation Study
- Physico-chemical Research Methods

8. Research interests

- Experimental and theoretical (molecular dynamics, quantum chemistry) study of inter-ion, ion-molecular and intermolecular interactions in molecular and ion-molecular systems, including acid-base equilibria and organized solutions.

9. Computational and programming experience

Experienced in operation systems: Windows and Linux based.
Experienced in using and installing computer software for carrying out computer modelling by using molecular dynamics simulations and ab initio quantum chemical calculations (GROMACS, NAMD, MOPAC, Gaussian, US GAMESS and PC GAMESS/Firefly).
Fluent in using and installing modern desktop office software.

10. PhD thesis defended under A.V. Lebed's supervision

1. Farafonov V. S. Localization and hydration of organic dyes in surfactant micelles by molecular dynamics simulations; Kharkiv, Ukraine, 2018.

11. Key publications (2017-2022, Scopus only)

1. V. S. Farafonov, **A. V. Lebed**. Developing and validating a set of all-atom potential models for sodium dodecyl sulfate // *J. Chem. Theory Comp.* –2017, – Vol.13, – P. 2742–2750.

DOI: 10.1021/acs.jctc.7b00181

2. V. S. Farafonov, **A. V. Lebed**, N. O. Mchedlov-Petrosyan. 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, – Vol.33, – P.8342–8352.

DOI: 10.1021/acs.langmuir.7b01737

3. V. S. Farafonov, **A. V. Lebed**, N. O. Mchedlov-Petrosyan. Solvatochromic betaine dyes of different hydrophobicity in ionic surfactant micelles: Molecular dynamics modeling of location character // *Colloids and Surfaces A.* –2018, – Vol.538, – P. 583-592.

DOI:10.1016/j.colsurfa.2017.11.046

4. N.O. Mchedlov-Petrosyan, V.S. Farafonov, **A.V. Lebed**. Examining surfactant micelles via acid-base indicators: Revisiting the pioneering Hartley–Roe 1940 study by molecular dynamics modeling // *J. Mol. Liq.* – 2018. –Vol. 264. – P. 683-690.

DOI:10.1016/j.molliq.2018.05.076

5. V.S. Farafonov, **A.V. Lebed**, N.O. Mchedlov-Petrosyan. Examining solvatochromic Reichardt's dye in cationic micelles of different size via molecular dynamics // *Voprosy khimii i khimicheskoi tekhnologii*, 2018, No. 5, pp. 62-68

6. N.O. Mchedlov-Petrosyan, V.S. Farafonov, T.A. Cheipesh, S.V. Shekhovtsov, D.A. Nerukh, **A.V. Lebed**. In search of an optimal acid-base indicator for examining surfactant micelles: Spectrophotometric studies and molecular dynamics simulations // *Colloids and Surfaces A.* – 2019, – Vol.565, – P. 97-107.

DOI:10.1016/j.colsurfa.2018.12.048

7. V. S. Farafonov, **A. V. Lebed**, N. O. Mchedlov-Petrosyan. Computing pKa shifts using traditional molecular dynamics: Example of acid-base indicator dyes in organized solutions. // *J. Chem. Theory Comput.* 2020. Vol. 16. No. 9. 5852–5865.

DOI:10.1021/acs.jctc.0c00231.

8. K. V. Gensh, Yu. E. Zevatskii, D.V. Samoylov, S.V. Shekhovtsov, **A. V. Lebed**, S.T. Goga, N.O. Mchedlov-Petrosyan. Ionic Equilibrium in Mixtures of Polar Protophobic and Protophilic Non-Hydrogen Bond Donor Solvents: Acids, Salts, and Indicators in Acetonitrile with 4 mass % Dimethylsulfoxide. // *J. Mol. Liquids*. 2021. V. 322. 114560.

DOI:10.1016/j.molliq.2020.114560

13. Linguistic ability: Native languages: Ukrainian, Russian

Other language proficiency on scale of 1 (basic) to 3 (fluent) for reading, writing and speaking: English 3, 3, 2;

14. Permanent private address

Yu. Gagarin Ave., 92, apt. 102,

Kharkiv-140, 61140, UKRAINE

Tel: +38 (066) 4127934

E-mail: alebed@karazin.ua

September, 2022