CURRICULUM VITAE

Ksenia B. Bravaya

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EDUCATION AND DEGREES

2008	Ph.D. in Theoretical and Computational Quantum Chemistry Department of Chemistry, Lomonosov Moscow State University, Russia
2005	B.Sc. and M.Sc. in Chemistry (with honors) Department of Chemistry, Lomonosov Moscow State University, Russia

APPOINTMENTS

2020 - current	Associate Professor, Department of Chemistry, Boston University
2013 - 2020	Assistant Professor, Department of Chemistry, Boston University
2009 - 2013	Postdoctoral Research Associate, Department of Chemistry, University of Southern California

HONORS AND AWARDS

2020	Alfred P. Sloan Research Fellowship Award
2017	Hariri Institute Research Award (BU)
2016	Patricia McLellan Leavitt Research Fund Award (BU)
2014	Hariri Institute Junior Faculty Fellow (BU)
2011	ACS Physical Chemistry Division Postdoctoral Research Award
2010	Burg Postdoctoral Teaching Award (USC)
2010	WISE Merit Award for Excellence in Postdoctoral Research (USC)

MANUSCRIPTS IN PROGRESS (*work completed*)

1. R.N Tazhigulov, J. Provazza, D.F. Coker, K.B. Bravaya; Photoactivation of cryptochromes invokes competing inter- and intra- molecular electron transfer, 2023 [Preprint is available at ChemRxiv].
2. S. Mondal and K.B. Bravaya; Complex potential energy surfaces with projected CAP technique: vibrational excitation of N_2, 2023.
3. J.R. Gayvert, A.J. Kranc, R.N. Tazhigulov, and K.B. Bravaya; eMap 2.0: A web-based platform for identifying electron transfer pathways in proteins and protein families, 2023.
4. M.G. Burrows and K.B. Bravaya; Redox potentials and reactivity of redox shuttles from polarizable QM/MM calculations, 2023.
5. V. Storozhilova and K.B. Bravaya; Charge transport through *Geobacter sulfurreducens* model e-pili: the role of protein fluctuations, 2023.

PUBLICATIONS *(total 46)*

1*. A.A. Kunitsa and K.B. Bravaya; *Feshbach projection XMCQDPT2 model for metastable electronic states* [Preprint is available at arXiv].

2*. J.R. Gayvert and K.B. Bravaya; OpenCAP: An Open-Source Framework for Computing Resonance Parameters in Molecules, J. Phys. Chem. A, 2023, submitted.

3*. J.R. Gayvert and K.B. Bravaya; Projected CAP-EOM-CCSD method for electronic resonances, J. Chem. Phys., 2022, 156, 094108.

4*. J.R. Gayvert and K.B. Bravaya; Application of Box and Voronoi CAPs for Metastable Electronic States in Molecular Clusters, J. Phys. Chem. A 2022, 126, 30, 5070–5078.

5*. E.A. Karnaukh and K.B. Bravaya; The Redox Potential of a Heme Cofactor in *Nitrosomonas europaea*: a Polarizable QM/MM Study, Phys. Chem. Chem. Phys., 2021, 23, 16506–16515.

6*. Y. Kim, Y. Bui, R.N. Tazhigulov, K.B. Bravaya, L.V. Slipchenko; Effective Fragment Potentials for Flexible Molecules: Transferability of Parameters and Amino Acid Database, J. Chem. Theor. Comp., 2020, 16, 7735–7747.

7*. Ragesh Kumar T.P., J. Kocisek, K.B. Bravaya, and J. Fedor; *Electron-induced vibrational excitation and dissociative electron attachment in methyl formate*, Phys. Chem. Chem. Phys., 2020, 22, 518–524.

8*. R.N. Tazhigulov, J.R. Gayvert, M. Wei, and K.B. Bravaya; *eMap: Web application for robust identification, mapping, and visualization of electron transfer channels in proteins*, J. Phys. Chem. B, 2019, 123, 6946–6951.

9*. R.N. Tazhigulov, P. Kumar Gurunathan, Y. Kim, L.V. Slipchenko and K.B. Bravaya; *Polarizable Embedding for Simulating Redox Potentials of Biomolecules*, Phys. Chem. Chem. Phys., 2019, 21, 11642–11650.

10*. Z. Li, M.M. Dawley, I. Carmichael, K.B. Bravaya, and S. Ptasińska; *Dipole-supported electronic resonances mediate electron-induced amide bond cleavage*, Phys. Rev. Lett., 2019, 22, 073002.

11*. M.K. Lee, K.B. Bravaya, and D.F. Coker; *First principles models for biological light-harvesting: Phycobiliprotein complexes from cryptophyte algae*, J. Am. Chem. Soc., 2017, 139, 7803–7814.

12*. A.A. Kunitsa, A.A. Granovsky, and K.B. Bravaya; *CAP-XMCQDPT2 method for molecular electronic resonances*, J. Chem. Phys., 2017, 146, 184107.

13*. T.C. Jagau, K.B. Bravaya, and A.I. Krylov; *Extending quantum chemistry of bound states to electronic resonances*, Ann. Rev. Phys. Chem., 2017, 68, 525–553.

14*. R.N. Tazhigulov and K.B. Bravaya; *Accurate redox half-reactions free energies from the first principle calculations*, J. Phys. Chem. Lett., 2016, 7, 2490–2495.

15*. A.A. Kunitsa and K.B. Bravaya; *Excited states electronic structure of the para-bezoquinone anion revisited*, Phys. Chem. Chem. Phys., 2016, 18, 3454–3462.

16*. A.A. Kunitsa and K.B. Bravaya; *First-principles calculations of the energy and width of the* ^2A_u *shape resonance in p-benzoquinone, a gateway state for electron transfer*, J. Phys. Chem. Lett., 2015, 6, 1053–1058.

17*. B.L. Yoder, K.B. Bravaya, A. Bodi, A.H.C. West, B. Sztáray, and R. Signorell; *Barrierless proton transfer across weak CH...O hydrogen bonds in dimethyl ether dimer*, J. Chem. Phys. 2015, 142, 114303.

18. A. Acharya, A. Bogdanov, B. Grigorenko, K. Bravaya, A. Nemukhin, K. Lukyanov, and A. Krylov *Photoinduced chemistry in fluorescent proteins: Curse or blessing?*, Chem. Rev., 2017, 117, 758–795.

19. A.M. Bogdanov, A.B. Kolomeisky, K.B. Bravaya, A. Acharya, A.V. Titelmayer, K.A. Lukyanov, and A.I. Krylov; *Turning on and off photoinduced electron transfer in fluorescent proteins by π-stacking, halide binding, and Tyr145 mutations*, J. Am. Chem. Soc., 2016, 138, 4807–4817.

20. Y. Shao, Z. Gan, E. Epifanovsky, A. TB Gilbert, M. Wormit, et al.; *Advances in molecular quantum chemistry contained in the Q-Chem 4 program package*, Mol. Phys., 2015, 113, 184–215.

21. V.A. Mironov, K.B. Bravaya, and A.V. Nemukhin; *On the role of zwitterions in kindling fluorescent protein photochemistry*, J. Phys. Chem. B, 2015, 119, 2467–2474.

22. J. Lazzari-Dean, A.I. Krylov, and K.B. Bravaya; *The effects of resonance delocalization and the extent of π-system on ionization energies of model fluorescent proteins chromophores*, Int. J. Quant. Chem., 2014,

115, 1258–1264
23. T.-C. Jagau, D. Zuev, K.B. Bravaya, E. Epifanovsky, Y. Shao, E. Sundstrom, M. Head-Gordon, A.I. Krylov; *Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks*, J. Chem. Phys. 2014, 141, 024102.
24. R.B. Vegh, K.B. Bravaya, D.A. Bloch, A.S. Bommarius, L.M. Tolbert, M. Verkhovsky, A.I. Krylov, K.M. Solntsev; *Chromophore photoreduction in red fluorescent proteins is responsible for bleaching and phototoxicity*, J. Phys. Chem. B 2014, 118, 4527–4534.
25. T.-C. Jagau, D. Zuev, K.B. Bravaya, E. Epifanovsky, A.I. Krylov; *A fresh look at resonances and complex absorbing potentials: density matrix-based approach*, J. Phys. Chem. Lett. 2014, 5, 310–315.
26. K.B. Bravaya and A.I. Krylov *On the photodetachment from the Green Fluorescent Protein chromophore*, J. Phys. Chem. A 2013, 117, 11815–11822.
27. K. Khistyaev, A. Golan, K.B. Bravaya, N. Orms, A.I. Krylov and M. Ahmed; *Proton transfer in nucleobases is mediated by water*, J. Phys. Chem. A 2013, 117, 6789–6797.
28. K.B. Bravaya, D. Zuev, A.I. Krylov; *Complex-scaled equation-of-motion coupled-cluster method with single and double substitutions for autoionizing excited states: Theory, implementation, and examples*, J. Chem. Phys. 2013, 138, 124106.
29. K.B. Bravaya, E. Epifanovsky, A.I. Krylov; *Four bases score a run: Ab initio calculations quantify a cooperative effect of h-bonding and pi-stacking on ionization energy of adenine in the AATT tetramer*, J. Phys. Chem. Lett. 2012, 3, 2726–2732.
30. B. Grigorenko, A.V. Nemukhin, D.I. Morozov, I. Polyakov, K.B. Bravaya, A.I. Krylov; *Towards molecular-level characterization of photo-induced decarboxylation of the green fluorescent protein: Accessibility of the charge-transfer states*, J. Chem. Theor. Chem. 2012, 8, 1912–1920.
31. A. Golan, K.B. Bravaya, R. Kudirka, O. Kostko, S.R. Leone, A.I. Krylov, M. Ahmed; *Ionization of dimethyluracil dimers leads to facile proton transfer in the absence of H-bonds*, Nat. Chemistry, 2012, 4, 323–329.
32. K.B. Bravaya, O.M. Subach, N. Korovina, V.V. Verkhusha and A.I. Krylov; *Insight into the common mechanism of the chromophore formation in the red fluorescent proteins: the elusive blue intermediate revealed*, J. Am. Chem. Soc. 2012, 134, 2807–2814.
33. K.B. Bravaya, B.L. Grigorenko, A.V. Nemukhin and A.I. Krylov; *Quantum chemistry behind bioimaging: Insights from ab initio studies of fluorescent proteins and their chromophores*, Acc. Chem. Res. 2012, 45, 265–275.
34. D. Zuev, K.B. Bravaya and A.I. Krylov; *Effect of microhydration on the electronic structure of the chromophores of the photoactive yellow and green fluorescent proteins*, J. Chem. Phys. 2011, 135, 194304.
35. K.B. Bravaya, M.G. Khrenova, B.L. Grigorenko, A.V. Nemukhin, and A.I. Krylov; *The effect of protein environment on electronically excited and ionized states of the green fluorescent protein chromophore*, J. Phys. Chem. B, 2011, 115, 8296–8303.
36. K. Khistyaev, K.B. Bravaya, E. Kamarchik, O. Kostko, M. Ahmed and A.I. Krylov; *The effect of microhydration on ionization energies of thymine*, Faraday Discussions, 2011, 150, 313–330.
37. D. Zuev, K.B. Bravaya, T. D. Crawford, R. Lindh and A.I. Krylov; *Electronic structure of the two isomers of the anionic form of p-coumaric acid chromophore*, J. Chem. Phys., 2011, 134, 034310.
38. K.B. Bravaya, O. Kostko, S. Dolgikh, A. Landau, M. Ahmed, and A.I. Krylov; *Electronic structure and spectroscopy of nucleic acid bases: Ionization energies, ionization-induced structural changes, and photoelectron spectra*, J. Phys. Chem. A, 2010, 114, 12305–12317.
39. K.B. Bravaya, O. Kostko, M. Ahmed and A.I. Krylov; *The effect of π-stacking, h-bonding, and electrostatic interactions on the ionization energies of nucleic acid bases: adenine-adenine, thymine-thymine and adenine-thymine dimers*, Phys. Chem. Chem. Phys., 2010, 12, 2292–2307.
40. O. Kostko, K.B. Bravaya, A.I. Krylov and M. Ahmed; *Ionization of cytosine monomer and dimer studied by VUV photoionization and electronic structure calculations.* Phys. Chem. Chem. Phys., 2010, 12, 2860–2872.
41. J. Rajput, D.B. Rahbek, L.H. Andersen, T. Rocha-Rinza, O. Christiansen, K.B. Bravaya, A.V. Erokhin, A.V. Bochenkova, K.M. Solntsev, J. Dong, J. Kowalik, L.M. Tolbert, M.A. Petersen and M.B. Nielsen;

Photoabsorption studies of neutral green fluorescent protein model chromophores in vacuo, Phys. Chem. Chem. Phys., 2009, 11, 9996–10002.

42. T. Rocha-Rinza, O. Christiansen, J. Rajput , A. Gopalan, D.B. Rahbek, L.H. Andersen, A.V. Bochenkova, A.A. Granovsky, K.B. Bravaya, A.V. Nemukhin, K.L. Christiansen and M.B. Nielsen; *Gas phase absorption studies of photoactive yellow protein chromophore derivatives*, J. Phys. Chem. A, 2009, 113, 9442–9449.
43. K.B. Bravaya, A.V. Bochenkova, A.A. Granovsky and A.V. Nemukhin; *Modeling photoabsorption of the asFP595 chromophore*, J. Phys. Chem. A 2008, 112, 8804–8810.
44. L. Kessel, I.B. Nielsen, A.V. Bochenkova, K.B. Bravaya and L.H. Andersen; *Gas-phase spectroscopy of protonated 3-OH kynurenine and argpyrimidine. Comparison of experimental results to theoretical modeling*, J. Phys. Chem. A 2007, 111, 10537–10543.
45. K.B. Bravaya, A.V. Bochenkova, A.A. Granovsky and A.V. Nemukhin; *An opsin shift in Rhodopsin: Retinal S_0-S_1 absorption in protein, in solution and in the gas phase*, J. Am. Chem. Soc. 2007, 129, 13035–13042.
46. K.B. Bravaya, A.V. Bochenkova, B.L. Grigorenko and A.V. Nemukhin; *Molecular modeling of reaction mechanism of serine-carboxyl peptidases*, J. Chem. Theor. Comp. 2006, 2, 1168–1175.

* - publications based on research conducted at BU

UPCOMING INVITED LECTURES

1. "QM/QM and Embedding Models", ACS Spring 2023 (March 26–30, Indianapolis, IN, 2023).
2. OpenMolcas developers meeting (virtual talk, June 13–June 16, 2023).
3. "Principles of light-induced charge transfer for optogenetics", CECAM workshop (July 3–5, Modena, Italy, 2023).
4. POSMOL 2023 (August 3–6, Notre Dame, IN, 2023).
5. "5th Conference of Theory and Applications of Computational Chemistry, TACC2020" (September 4–9, Sapporo, Japan, 2023).

INVITED CONFERENCE TALKS

1. "International Conference on Molecular Electronic Structure" (virtual talk, September 02–06, 2022).
2. "Quantum Chemistry: Current and Future Frontiers", ACS Fall 2022 (August 21–25, Chicago, IL, 2022).
3. WATOC 2020 (postponed due to COVID) (July 3–8, Vancouver, Canada, 2022).
4. "The Synergy of Theory and Experiment: A Symposium in Honor of Prof. John F. Stanton" (March 20–24, San Diego, CA, 2022).
5. "Theory and Simulation of Electronic and Optical Processes in Molecules and Materials" virtual seminar series (virtual talk, November 3, 2021).
6. "Orbital Models in Electronic Structure Theory" symposium, ACS Fall 2021 (virtual talk, August 22–26, 2021).
7. "Advanced Force Field" symposium", ACS Fall 2021 (virtual talk, August 22–24, 2021).
8. "Advances in theory of electronic resonances", TSRC workshop (virtual talk, July 13–17, 2021).
9. "Virtual New Frontiers in Electron Correlation" TSRC workshop (virtual talk, June 14–18, 2021).
10. "Virtual Warsaw Molecular Electronic Structure Conference" (virtual talk, September 1st, 2020).
11. "Developments in QM/MM and Embedding models for Photochemical and Electron Transfer Processes" TSRC workshop (virtual talk, July 30th, 2020).
12. "Utah Workshop on Methods and Applications in Molecular and Solid State Theory" (September 22-27, Salt Lake City, UT, 2019).
13. "Frontiers in multiscale modeling of photoreceptor proteins (September 3–5, Tel Aviv, Israel, 2019).
14. "Interface between experiments and modeling in unraveling the physical and chemical properties of charged droplet" symposium, 258th ACS meeting (August 25–29, San Diego, CA, 2019).
15. "Symposium in Honor of Fritz Schaefer", 258th ACS meeting (August 25–29, San Diego, CA, 2019).

16. "Advances in Theory of Electronic Resonances" workshop (July 22–26, Telluride, CO, 2019).
17. ISTCP-X congress (July 11–17, Tromsø, Norway, 2019).
18. 9th Molecular Quantum Mechanics conference (June 30–July 5, Heidelberg, Germany, 2019).
19. "New Frontiers in Electron Correlation" workshop (June 10–14, Telluride, CO, 2019).
20. "Electronic Structure Theory: New Models and Challenging Applications" symposium, 102nd Canadian Chemistry Conference and Exhibition (June 3–9, Quebec, Canada, 2019).
21. "Modeling Dynamics in Dense Manifolds of Electronic States" symposium, 257th ACS meeting (March 31–April 4, Orlando, FL, 2019).
22. "Electron-molecule and molecule-molecule interaction" symposium, 257th ACS meeting (March 31–April 4, Orlando, FL, 2019).
23. Pacific Conference on Spectroscopy and Dynamics (January 24–29, San Diego, CA, 2019).
24. Molecular Electronic Structure (August 28–31, Metz, France, 2018).
25. Developments in QM/MM and Embedding Models for Photochemical and Electron Transfer Processes (July 09–13, Telluride, CO, 2018).
26. Penn Conference in Theoretical Chemistry (June 10–14, Philadelphia, PA, 2018).
27. New Developments in Coupled-Cluster Theory (July 31 – August 4, Telluride, CO, 2017).
28. Advances in theory of electronic resonances (July 17–21, Telluride, CO, 2017).
29. New Frontiers in Electron Correlation (June 19–24, Telluride, CO, 2017).
30. "Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities" symposium, 253rd ACS meeting (April 2-6, San Francisco, CA, 2017).
31. Molecular Electronic Structure - Buenos-Aires (September 19 - September 23, Buenos-Aires, Argentina, 2016).
32. "Advanced Potential Energy Surfaces Symposium" symposium, 252nd ACS meeting (August 21–25, Philadelphia, PA, 2016).
33. ISTCP IX conference (July 17–22, Grand Forks, ND, 2016).
34. 23rd Conference on Current Trends in Computational Chemistry (November 13–14, Jackson, MS, 2015).
35. New Developments in Coupled-Cluster Theory (August 3–7, Telluride, CO, 2015).
36. Advances in theory of electronic resonances: A workshop in honor of Howard Taylor (July 20–24, Telluride, CO, 2015).
37. Modeling Photoactive Molecules conferences (Nantes, April 21–24, Nantes, France, 2015).
38. Department of Physics, University of Massachusetts Boston (Oct. 16, Boston, MA, 2014).
39. Molecular Electronic Structure (Sep. 1–5, Amasya, Turkey, 2014).
40. "The Future of Computational Chemistry" symposium, 248th ACS meeting (Aug. 10–14, San Francisco, CA, 2014).
41. "Excited States and Time-Dependent Electronic Structure Theory" (Jul. 14–18, Telluride, CO, 2014).
42. "Spectroscopy and dynamics on multiple potential surfaces", (Jul. 7–11, Telluride, CO, 2014).
43. Tensor workshop (Dec. 8–11, Laguna Beach, CA, 2013).
44. SERMACS 2013 (Nov. 12–16, Atlanta, GA, 2013).
45. Q-Chem developer workshop (Sep. 7, Indianapolis, IN, 2013).

INVITED UNIVERSITY SEMINARS AND LECTURES

1. Department of Chemistry, University of Massachusetts Dartmouth (October 20, North Dartmouth, MA, 2021).
2. Department of Chemistry, California Institute of Technology (March 4, Pasadena, CA, 2019).
3. Department of Chemistry, Purdue University (November 28, West Lafayette, IN, 2018).
4. Department of Chemistry, Virginia Tech (November 30, Blacksburg, VA, 2018).
5. Department of Chemistry, University of Washington (October 17, Seattle, WA, 2018).
6. Department of Chemistry, Rice University (October 3, Houston, TX, 2018).

7. Department of Chemistry, University of Utah (October 1, Salt Lake City, UT, 2018).
8. Department of Chemistry, Lomonosov Moscow State University (September 14, Moscow, Russia, 2018).
9. Department of Chemistry, Georgia Institute of Technology (September 6, Atlanta, GA, 2018).
10. Department of Chemistry, University of Toronto (March 6, Toronto, Canada, 2018)
11. Department of Chemistry, Brown University (October 19, Providence, RI, 2017).
12. Department of Physics, Northeastern University (November 6, Boston, MA, 2016).
13. Department of Chemistry, Clark University (April 15, Worcester, MA, 2016).
14. Greater Boston Area Theoretical Chemistry Lecture Series, Boston University - MIT - Harvard (April 6, Boston, MA, 2016).
15. Department of Chemistry, Bowling Green State University (February 10, Bowling Green, OH, 2016).
16. Department of Physics, University of Massachusetts Boston (November 5, Boston, MA, 2015).
17. Department of Physics and Astronomy, Aarhus University (April 17, Aarhus, Denmark, 2015).
18. Department of Chemistry, Colby College (Feb. 13, Waterville, ME, 2015).

RESEARCH SUPPORT (*funded*)

1. National Institute Of General Medical Sciences of the National Institutes of Health, SBIR, Phase II: *Algorithmic improvements in large scale polarizable QM/MM simulations*; R44 GM126804-02A1, 8/1/2022 – 7/31/2024, $250,000 (*co-PI*).
2. Alfred P. Sloan Foundation: *Alfred P. Sloan Research Fellowship*, 09/15/2020 - 09/14/2022, $75,000 (*PI*).
3. Department of Energy: *Control of Energy Transport and Transduction in Photosynthetic Down-Conversion,* DE-SC0020437, 09/15/2019 – 09/14/2022, $99,189 (*co-PI*).
4. Army Research Office: *Non-Hermitian Quantum Mechanics for Chemistry and Catalysis,* 71010-CH; 01/01/2019 – 12/31/2021, $579,033 (*PI*).
5. National Institute Of General Medical Sciences of the National Institutes of Health, SBIR, Phase I: *Algorithmic improvements in large scale polarizable QM/MM simulations;* R43 GM126804; 01/01/2019 – 05/31/2019, $45,000 (*co-PI*).
6. National Science Foundation: *Metastable electronic states: Electronic structure, dynamics, and chemistry;* CHE-1665276, 06/01/2017 – 05/31/2020, $405,000 (*PI*).
7. Hariri Institute for Computational Science & Engineering (BU): *eMap: Online mapping electron transfer channels in proteins;* #2016-10-003, 06/01/2017 – 05/31/2018, $15,000 (*PI*).

PROFESSIONAL ACTIVITIES

Conference organization: "Advances in theory of electronic resonances" (Telluride, CO, July 22-26, 2019); "Advances in theory of electronic resonances" (Telluride, CO, July 17-21, 2017); ACS symposium "Metastable electronic states: recent advances in theory and experiment" (San Diego, CA, March 13-17, 2016); Q-Chem Developers' meeting (Boston, MA, August 21-22, 2015); TSRC workshop "Advances in theory of electronic resonances: A workshop in honor of Howard Taylor" (Telluride, CO, July 20-24, 2015).
Referee/reviewer for: Computational and Theoretical Chemistry, The Journal of Chemical Physics, Theoretical Chemistry Accounts, Journal of Chemical Theory and Computations, Physical Review Letters, Chemical Sciences, The New Journal of Chemistry; National Science Foundation, Department of Energy, ACS Petroleum Research Fund.
Program panelist for: National Science Foundation, Department of Energy.