Yevhen HORBATENKO

Birth Date: October 6, 1985
Birth Place: Sumy, Ukraine
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Skills

- good knowledge of electronic structure theory;
- good knowledge of molecular vibration theory;
- good knowledge of organic, organometallic, and inorganic chemistry;
- good knowledge of photochemistry and photophysics;
- programming skills;
- languages: English (fluent), Spanish (fluent), Russian (native), Ukrainian (native);

Programming languages and software packages:

- Fortran 77/90/95, Python, Bash, C Shell, Awk, Sed, Vim, Gnuplot, LaTeX;
- MOLPRO 2019.2, GAMESS-US 2014/2017/2018/2020, VASP 5.3, Quantum Espresso 5.2, Gaussian 03/09/13, Turbomole 5.10, Cfour, Orca 2.8.0, ADF 2012.01;

Academic and professional appointments

09/2022 – present **Research professor, IBS Center for Spectroscopy and Molecular Dynamics, R&D Center at Korea University, Seoul, Republic of Korea**
Host: Prof. S. Ringe

04/2017 – 03/2021 **Research professor, Kyungpook National University, Chemistry Department, Daegu, Republic of Korea**
Host: Prof. C. H. Choi

04/2014 – 03/2017 **Research fellow, IBS Center for Multidimensional Carbon Materials, Ulsan, Republic of Korea**
Host: Prof. N. Park

Education

11/2009 – 12/2013 **Doctorate in Theoretical and Computational Chemistry, University of Girona, Spain**
Thesis Title: "Structure and Hydrogen Dynamic Behavior in Proton Sponge Cations and Organometallic Complexes"
Supervisor: Prof. S. F. Vyboishchikov
Reading Committee: Prof. G. Frenking, Prof. F. Maseras, Prof. M. Solà

10/2008 – 11/2009 **Master in Theoretical and Computational Chemistry, University of Tarragona, Spain**
Master Title: "Proton Behavior in Proton Sponges: A Theoretical Study"
Supervisor: Prof. S. F. Vyboishchikov

09/2002 – 06/2007 **Diploma (=M.Sc.) in Organic Chemistry, Lomonosov Moscow State University, Russia**
Diploma Title: "Synthesis and NMR Spectra of Indole-^{15}N and Quinoline-^{15}N"
Supervisor: Dr. V. A. Chertkov

Awards

Polar Research Institute affiliated with Korea Institute of Ocean Science and Technology Grant (PE21120, Participant 2018 – 2021, Host: Prof. C. H. Choi 2018 – 2022, Total: about 265,000$)

Samsung Future Technology Promotion Foundation Grant (SSTF-BA1701-12, Participant 2017 – 2021, Host: Prof. C. H. Choi 2017 – 2022, Total: about 1,300,000$)

Graduate Fellowship (BR08/02) of the University of Girona, Spain (06/2008 – 06/2012).

Fellowship of "ChemBridge" Corporation for the best participants in Organic Chemistry Olympiad for students and young scientists, Moscow State University, Russia (09/2006 – 05/ 2007).

Participant of "ChemBridge" Corporation Olympiad in Organic Chemistry for students and young scientists, Moscow State University, Russia, 2007 (position 31 out of 111), 2006 (position 14 out of 121), 2005 (position 14 out of 85).

Publications

- **Yevhen Horbatenko** and Sergei F. Vyboishchikov *"Hydrogen motion in proton sponge cations: a theoretical study"* ChemPhysChem, 2011, **12**, 1118-1129.

- **Yevhen Horbatenko** and Sergei F. Vyboishchikov *"Dynamic behavior of hydrogen in transition metal bis(silyl)hydride complexes"* Organometallics, 2013, **32**, 514-526.

- **Yevhen Horbatenko** and Sergei F. Vyboishchikov *"Si···H interligand interactions in cobalt(V) and iridium(V) bis(silyl)bis(hydride) complexes"* ChemPlusChem, 2013, **78**, 1073-1081. (Special issue in memory of Detlef Schröder)

- **Yevhen Horbatenko**, Juan Pedro Pérez, Pedro Hernández, Marcel Swart, Miquel Solà *"Reaction mechanisms for the formation of mono- and dipropylene glycol from the propylene oxide hydrolysis over ZSM-5 zeolite"* J. Phys. Chem. C, 2014, **118**, 21952-21962.

- **Yevhen Horbatenko**, Min Choi, Rodney S. Ruoff, Christopher W. Bielawski, and Noejung Park *"First-principles investigation of wet-chemical routes for the hydrogenation of graphene"* Carbon, 2015, **93**, 421-430.

- **Yevhen Horbatenko**, Masood Yousaf, Jihyung Lee, Tae Hoon Choi, Rodney S. Ruoff, and Noejung Park *"Synergetic interplay between pressure and surface chemistry for the conversion of sp^2-bonded carbon layers into sp^3-bonded carbon films"* Carbon, 2016, **106**, 158-163.

- Pramoda K. Nayak, **Yevhen Horbatenko**, Seongjoon Ahn, Gwangwoo Kim, Jae-Ung Lee, Kyung Yeol Ma, A-Rang Jang, Hyunseob Lim, Dogyeong Kim, Sunmin Ryu, Hyeonsik Cheong, Noejung Park, and Hyeon Suk Shin *"Probing evolution of twist-angle-dependent interlayer excitons in $MoSe_2/WSe_2$ van der Waals Heterostructures"* ACS Nano, 2017, **11**, 4041-4050.

- **Yevhen Horbatenko**, Dongbin Shin, Sang Soo Han, and Noejung Park *"Excitation-driven non-thermal conversion of few-layer graphenes into sp^3-bonded carbon nanofilms"* Chem. Phys. Lett., 2018, **694**, 23-28.

- **Yevhen Horbatenko**, Seunghoon Lee, Michael Filatov, Cheol Ho Choi *"Performance Analysis and Optimization of Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) for Vertical Excitation Energies and Singlet–Triplet Energy Gaps"* J. Phys. Chem. A, 2019, **123**, 7991-8000.

- Svetlana Shostak, Kitae Kim, **Yevhen Horbatenko**, Cheol Ho Choi *"Sulfuric Acid Formation via H_2SO_3 Oxidation by H_2O_2 in the Atmosphere"* J. Phys. Chem. A, 2019, **123**, 8385-8390.

- **Yevhen Horbatenko**, Seunghoon Lee, Michael Filatov, Cheol Ho Choi "*How Beneficial is the Explicit Account of Doubly Excited Configurations in Linear Response Theory?*" J. Chem. Theory Comput. 2021, **17**, 975-984.

- **Yevhen Horbatenko**, Saima Sadiq, Seunghoon Lee, Michael Filatov, Cheol Ho Choi "*Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory (MRSF-TDDFT) as a Simple yet Accurate Method for Diradicals and Diradicaloids*" J. Chem. Theory Comput. 2021, **17**, 848-859.

- Seunghoon Lee, **Yevhen Horbatenko**, Michael Filatov, Cheol Ho Choi "*Fast and Accurate Computation of Nonadiabatic Coupling Matrix Elements using the Truncated Leibniz Formula and Mixed-Reference Spin-Flip Time-Dependent Density Functional Theory*" J. Phys. Chem. Lett. 2021, **12**, 4722-4728.

- **Yevhen Horbatenko**, Nizam Uddin, Cheol Ho Choi "*New insight into origin of Zundel continuum observed in IR spectra of protonated water clusters*", in preparation.

Conference presentations

Authors: Y. Horbatenko, S. Lee, M. Filatov, C. H. Choi "MRSF-TDDFT benchmarks for Vertical Excitation Energies and Singlet-Triplet Energy Gaps." ***(oral communication)***
Conference: 130th KCS summer symposium in physical chemistry (Busan, Korea, 8–10 July 2019)

Authors: Y. Horbatenko, C. H. Choi "Origin of high reactivity and enhanced endo/exo selectivity in water-accelerated Diels-Alder reactions" (poster)
Conference: 123rd General meeting of the Korean Chemical Society (Suwon, Korea, 17–19 April 2019)

Authors: Y. Horbatenko, C. H. Choi "Origin of Zundel broadening explained via particular vibrational modes of Eigen structure altered by solvent environmental effects" ***(oral communication)***
Conference: 122nd General meeting of the Korean Chemical Society (Daegu, Korea, 17–19 October 2018)

Authors: S. Shostak, **Y. Horbatenko**, C. H. Choi "Mechanism of the oxidation of sulfurous acid by hydrogen peroxide" (poster)
Conference: 2nd SNU workshop on ice chemistry and physics (Seoul, Korea, 16 July 2018)

Authors: N. Uddin, **Y. Horbatenko**, C. H. Choi "Origin of Zundel broadening explained via stretching vibrational modes of hydronium altered by environmental effects" (poster)
Conference: 127th Korean Chemical Society Meeting (KCS) (Sokcho, Korea, 9–11 July 2018)

Authors: Y. Horbatenko, M. Yousaf, R. S. Ruoff, J. Lee, T. H. Choi, N. Park "Concerted interplay between pressure and surface chemistry as a way for the conversion of few graphene layers into nanodiamond" ***(oral communication)***
Conference: 10th International Conference on New Diamond and Nano Carbons (NDNC) (Xian, China, 22–26 May 2016)

Authors: Y. Horbatenko, M. Choi, R. S. Ruoff, Ch. W. Bielawski, N. Park "First-principles investigation of novel chemical routes for the efficient graphene hydrogenation" (poster)
Conference: 10th International Conference on New Diamond and Nano Carbons (NDNC) (Xian, China, 22–26 May 2016)

Authors: Y. Horbatenko, M. Choi, N. Park "Novel chemical routes for efficient graphene hydrogenation: A theoretical study" (poster)
Conference: The 20th Nanotube Conference (Muju, Republic of Korea, 29–31 Jan 2015)

Authors: Y. Horbatenko, M. Choi, N. Park "Ab initio exploration of possible chemical routes for efficient high coverage graphene hydrogenation" (poster)
Conference: The 5th A3 Symposium on Emerging Materials: sp^2 Nanocarbon for Energy 2014 (Tianjin, China, 19–21 Oct 2014)

Authors: Y. Horbatenko, S. F. Vyboishchikov "Hydrogen behavior in Si···H···Si organometallic complexes" (poster)
Conference: X Girona Seminar on Theoretical and Computational Chemistry for the Modeling of Biochemical Systems: From Theory to Applications (Girona, Spain, 2–5 Jul 2012)

Authors: Y. Horbatenko, S. F. Vyboishchikov "Si···H···Si interligand interactions in organometallic complexes" (poster)
Conference: World Association of Theoretical and Computational Chemists (WATOC) (Santiago de Compostela, Spain, 17–22 Jul 2011)

Authors: Y. Horbatenko, S. F. Vyboishchikov "Hydrogen behavior in proton sponges" ***(oral communication)***
Conference: XXVII Reunió de la XARXA de referència de Química Teòrica i Computacional de Catalunya (XRQTC) (Tarragona, Spain, 21–22 Jun 2011)

Authors: Y. Horbatenko, S. F. Vyboishchikov "Hydrogen motion in proton sponges" (poster)

Conference: 8th European Conference on Computational Chemistry (EUCO-CC) (Lund, Sweden, 25–28 Aug 2010)

Authors: Y. Horbatenko, S. F. Vyboishchikov "Hydrogen motion in proton sponges" ***(oral communication)***
Conference: IX Girona Seminar. Electron density, Density matrices, and Density Functional Theory (Girona, Spain, 5–8 Jul 2010)

Authors: Y. Horbatenko, S. F. Vyboishchikov "Shape of energy surfaces for N···H···N hydrogen bonds" (poster)
Conference: International Symposium on Theoretical and Computational Chemistry (Mülheim an der Ruhr, Germany, 28 Feb–2 Mar 2010)

Authors: Y. Horbatenko, S. F. Vyboishchikov "The shape of potential energy surfaces for NHN hydrogen bonds" (poster)
Conference: XXV Reunió de la XARXA de referència de Química Teòrica i Computacional de Catalunya (XRQTC) (Barcelona, Spain, 29 Jun–3 Jul 2009)

Authors: Y. Horbatenko, O. V. Smirnova, A. K. Shestakova, A. V. Chertkov "Synthesis and NMR spectra of indole-^{15}N and quinoline-^{15}N" (poster)
Conference: Magnetic Resonance and its Applications (St. Petersburg, Russia, 3–7 Dec 2007)

Nuclear Magnetic Resonance summer school, Moscow, Russia (17–19 Jun 2007)

Students Mentoring

Saima Sadiq (M.Sc. student, KNU, 2020 – 2021): Y. Horbatenko, S. Sadiq, S. H. Lee, M. Filatov, C. H. Choi J. Chem. Theory Comput. 2021, **17**, 848-859.

Svetlana Shostak (M.Sc. student, KNU, 2018 – 2019): S. Shostak, K. T. Kim, Y. Horbatenko, C. H. Choi J. Phys. Chem. A, 2019, **123**, 8385-8390.

Guiding various B.Sc. students during a research fellow contract (IBS, 2014 – 2017) and a research professor contract (KNU, 2017 – 2021).

Industrial Projects

02/2013 – 08/2013 Computational chemistry applied to catalysis: design of a heterogeneous catalyst for synthesis of the propylene glycol. (Funding body: REPSOL Corporation, Spain)

Research Stays

10/2010 – 12/2010	**University of Yamanashi, Fuel Cell Nanomaterials Center, Kofu, Japan** **Application of vibrational SCF, MP2, and CI to proton sponge cations** **Host:** Prof. K. Yagi
09/2007 – 12/2007	**Lomonosov Moscow State University, Chemistry Department Moscow, Russia** **Synthesis of isoquinoline-^{15}N** **Host:** Dr. V. A. Chertkov

Scientific Interests

- 2D nanomaterials;
- Solid-liquid (electrified) interfaces;
- Machine learning in application for new materials design;
- Solvation effects;
- Multiscale modeling

Referees

Cheol Ho Choi
Full Professor

Noejung Park
Department Chair Professor

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Work Experience and Major Achievements

Kyungpook National University

Jul 2020 – present **Origin of double fluorescence in DMABN via excited state non-adiabatic MD simulations.**

- a working hypothesis is that the double fluorescence arises from various vibrationally distorted structures rather than planar and twisted as discussed in the literature;
- previously unknown conical intersection that is expected to play a role into the ultrafast relaxation process of DMABN was found;

Dec 2019 – Mar 2021 **Accurate calculations of the first-order non-adiabatic coupling matrix elements with MRSF-TDDFT for non-adiabatic molecular dynamics for simulation of potential solar energy harvesting and conversion materials as well as OLED devices.**

- an excellent accuracy of MRSF-TDDFT for calculations of the first-order non-adiabatic coupling matrix elements (NACME) was demonstrated;
- MRSF-TDDFT described accurately and correctly not only NACME between the ground and excited states of H_2 but also the much more difficult to obtain NACME between the two excited states;
- the method accurately describes avoided crossing regions between the electronic states as compared with FCI dissociation curves;
- a close agreement between MRSF and the MRCISD NAC vectors for the case of polyatomic molecules was shown;

Apr 2017 – Jul 2020 **QM/MM molecular dynamics study of origin of Zundel continuum band in IR spectra of aqueous acid solutions.**

- the origin of Zundel continuum was investigated by molecular dynamics performed on Eigen and Zundel models embedded in either ice or liquid water environments;
- it was found that the continuum originates from three particular O-H stretching modes of the Eigen entity;
- the stretching modes are shifted and further broadened by two environmental effects: the short-range thermal fluctuations by the second solvation shell and the long-range electrostatic interactions between Eigen's positive charge and the polar medium.

Sept 2019 – Oct 2020 **MRSF-TDDFT as a simple and accurate method for diradical(oid) challenging systems for singlet fission in solar energy harvesting and for OLED devices.**

- as found, MRSF-TDDFT is capable of describing the multi-configurational electronic nature, accurate singlet-triplet gaps, the Jahn-Teller distortion, the violation of the Hund rule, and the potential energy surface of diradical(oid)s, systems where common LR- and SF-TDDFT theories fail;
- convenient criterium to distinguish between diradicals and diradicaloidis on the basis of easily obtainable quantities was suggested;

Sept 2019 – Oct 2020 **MRSF-TDDFT as a method of choice for an accurate description of doubly-excited configurations for photosynthesis implications.**

- the importance of the explicit account of double excitations in polyenes was investigated;
- it was shown MRSF-TDDFT can flexibly take both an implicit (through the XC functional) and an explicit (through double excitations) accounts of the electron correlation providing a more balanced description of various types of the excited states regardless of their character;

May 2018 – Aug 2019 **Atmospheric oxidation mechanism of H_2SO_3 by H_2O_2.**

- it was found that addition of one water molecule exhibits a strong catalytic effect that dramatically reduces the overall reaction barrier in comparison to gas phase;
- oxidation occurs via peroxo-intermediates: previously unknown $(HOO)S(OH)_3$ intermediate was discovered;
- a rearrangement step of $(HOO)SO_2^-$ intermediate to HSO_4^- found earlier in experiments was revealed;

Jul 2018 – Aug 2019 Optimization of the MRSF-TDDFT method for the calculations of the vertical excitation energies and the singlet−triplet gaps for OPV and OLED devices.

- the dependence of the excitation energies and singlet-triplet gaps on the intrinsic parameters of the method were investigated and prescriptions for the method use were formulated;
- a better accuracy of MRSF-TDDFT for excitation energies and singlet-triplet gaps than that of SF-TDDFT and LR-TDDFT was shown;

IBS Center for Multidimensional Carbon Materials

Sept 2015 – Mar 2017 Excited state non-adiabatic dynamics study of femtosecond control of carbon phases: Excitation-induced sp^2 (graphene) to sp^3 (nanodiamond) transformation.

- the effect of hole doping and femtosecond laser irradiation on the conversion of ABC-stacked graphite to bulk diamond was investigated;
- the dependence of the transformation barrier on the concentration of holes as well as excited electrons was demonstrated;
- a possibility of the conversion of graphene bilayer to sp^3 carbon nanofilms through dynamical hole doping in the presence of acceptors of excited elections was shown;
- it was found that not only molecules but also a (111) surface of a face-centered cubic transition metal separated by an insulating layer can serve as acceptor of excited electrons;

Sept 2015 – Aug 2016 Dependence of interlayer exciton on twist angle in $MoSe_2/WSe_2$ heterostructures.

- interlayer exciton evolution in $MoSe_2/WSe_2$ heterobilayer structures with respect to a twist angle between the two layers was revealed;
- it was found that the intensity of the emission peaks during photoluminescence was the strongest at 0° and 60°, and largely diminished at the intermediate angles;
- the dependence of the intensity of the emission peaks on the twist angle in terms of orbital mixing between two layers was explained;
- the hypothesis was supported by the results of the Raman analysis;

Jan 2015 – Aug 2015 Interplay between pressure and surface chemistry for the conversion of sp^2 carbon layers into sp^3 nanodamond carbon films.

- importance of surface chemistry for the conversion of few graphene layers was demonstrated;
- N_2H_4 and H_2O were demonstrated to serve as hydrogen donors that stabilized sp^3 carbon film by functionalizing its outer surface;
- ability to reduce a conversion pressure value was found for the hydrogen donors in comparison with inert medium (He);

Apr 2014 – Feb 2015 Investigation of wet-chemical routes for the graphene hydrogenation.

- microscopic mechanism for the Birch-type hydrogenation of graphene was investigated;
- the role of alkali atoms (e^- donor) when CH_3OH (H donor) is used was demonstrated;
- better reaction thermodynamics for $CH_3NH_3^+$ salts (H donor) was shown;
- an experimental setup with metal electrode instead of alkali atoms was suggested;

University of Girona

Dec 2012 – Jul 2013 Si···H interactions in Co(V) and Ir(V) bis(silyl)bis(hydride) complexes.

- various residual Si···H interactions in Co(V) complexes were detected;
- absence of residual Si···H interactions in Ir(V) complexes was demonstrated;

Apr 2011 – Dec 2012 Hydride dynamic behavior in organorhodium complexes.

- asymmetric arrangement and simultaneous interactions of hydride with two silyl ligands were demonstrated;
- 3-dimensional vibrational Schrödinger equation was solved;
- 3-dimensional ground-state vibrational wavefunctions were analyzed;
- criterion for localized and delocalized hydride behavior in Rh complexes was proposed;
- influence of vibrational motion of hydride on J(Si–H) coupling constants was demonstrated;

Sep 2009 – Apr 2011 Proton dynamic behavior in proton sponge cations.

- 3-dimensional vibrational Hamiltonian matrix elements were derived;
- 3-dimensional linear least-squares method was derived;
- Fortran-90 code for 3-dimensional vibrational problem was co-developed;
- 3-dimensional vibrational Schrödinger equation was solved;
- 3-dimensional ground-state vibrational wavefunctions were analyzed;
- criterion for localized and delocalized proton behavior in proton sponges was proposed;
- description of vibrational excited states in terms of particle-in-a-box model was proposed;

Oct 2010 – Dec 2010 (*Short research stay*) Application of vibrational SCF, MP2, and CI to proton sponge cations.

- theory of quartic force field representation of potential energy surface was studied;
- theory of vibrational methods was studied;
- Fortran-90 code for selection of vibrational modes was co-developed;
- vibrational methods were applied to proton sponge cations;
- vibrational frequencies were compared to those from vibrational Schrödinger equation;
- vibrational methods were applied to N-methylacetamide to reproduce the Fermi resonance;

Lomonosov Moscow State University

Sep 2007 – Dec 2007 (*Short Research Stay*) Synthesis of isoquinoline-^{15}N.

- ^{15}N NMR spectra of isoquinoline-^{15}N were *obtained for the first time*;
- spin-spin coupling constants (^{1}H-^{1}H, ^{15}N-^{1}H) were determined;

Oct 2006 – May 2007 Synthesis, analysis (NMR, *ab initio* calculations) and orientation effects of quinoline-^{15}N and indole-^{15}N in strong magnetic fields.

- orientation effects of aromatic molecules in strong magnetic fields were studied;
- ^{15}N NMR spectra of indole-^{15}N and quinoline-^{15}N were *obtained for the first time*;
- spin-spin coupling constants (^{1}H-^{1}H, ^{15}N-^{1}H, ^{13}C-^{1}H) were determined;
- dipole-dipole coupling constants of these molecules were obtained;

Dec 2005 – May 2006 Analysis of 2'-deoxyadenosine conformations.

- quantum-mechanical calculations of spin-spin coupling constants were done;
- potential energy surface for sugar conversion C2'-*endo* into C3'-*endo* was obtained;
- intramolecular hydrogen bond was found based on NMR spectrum;

Nov 2004 – May 2005 Conformational analysis of cyclobutane derivatives.

- 1-bromocyclobutanecarbonitrile synthesis and identification (NMR) were performed;
- conformational analysis was done;

Nov 2003 – May 2004 Spectrophotometric determination of Co in vitamin B_{12}.

- optimal spectral characteristics of Co complex salt were studied;
- technique for Co determination in pharmaceutical samples was developed;

Nov 2002 – May 2003 Synthesis and characterization of La complexes with organic ligands.

- La trifluoroacetylacetonate was synthesized and its volatility was determined;