Jacek **Klos**

Ph. D. · Chemistry

Department of Chemistry & Biochemistry, University of Maryland, College Park MD 20742 USA

(+1) 301-375-0115(cell), 301-405-1384 (office) | jklos@umd.edu | www.researcherid.com/rid/A-6457-2008

"My career objective is to continue my research and teaching career in the academic setting. Create successful internationally recognized research program that attracts extra-mural funding. Create novel and interesting courses for students."

Education

Department of Chemistry, University of Warsaw — *Warsaw, Poland*

Ph. D. in Chemistry — *Oct. 1997-Dec. 2001*

- Thesis: "Van der Waals complexes containing open-shell monomers"
- Advisor: Prof. G. Chalasinski

Department of Chemistry, University of Warsaw — *Warsaw, Poland*

M. Sc. in Chemistry — *Oct. 1992-Jun. 1997*

- Thesis: "*Ab initio* studies of the interaction of He with the NO($X^2\Pi$)"
- Advisor: Prof. G. Chalasinski

Technical Chemical Secondary School — *Warsaw, Poland*

Technical Diploma of Analytical Chemist — *May. 1987-Jun. 1992*

- Specialization diploma: "Gas chromatography of flavonoids and terpenoids in aromatic oils"

Academic Experience

Department of Chemistry & Biochemistry, University of Maryland — *College Park, MD*

Research Assistant Professor — *Dec. 2009 - Present*

- Research in the field of *ab initio* calculations and dynamics of open-shell systems, preparation of manuscripts for publications.
- Developed potential energy surfaces for ground and excited states of SO_2 molecule for NASA Astrobiology project.
- Developed and modeled potential energy surfaces for OH and NO radicals (both ground X and excited A states) with rare gases and hydrogen molecule.
- Spectra and scattering simulations, collaborations with two experimental groups, laser and carbon nanotubes groups.
- Developed, from scratch, and taught computational chemistry course. Installed WebMO Pro servers and linked with Gaussian and Molpro software.

Department of Chemistry & Biochemistry, University of Maryland — *College Park, MD*

Postdoctoral Research Associate — *Aug. 2004 - Dec. 2009*

- Research in the field of *ab initio* calculations and dynamics of open-shell systems.
- Taught physical chemistry laboratory course (CHEM-484).
- Advisor: Prof. Millard Alexander

Department of Chemistry, Oakland University — *Rochester Hills, MI*

Short-term Postdoctoral Scholar — *Mar. 2004 - Jul. 2004*

- Developed potential energy curves for transition metal atoms with He atom.
- *Ab initio* calculations of tensor polarizabilities of transition metal atoms.
- Advisor: Prof. M. M. Szczesniak

Department of Chemistry, Complutense University — *Madrid, Spain*

Postdoctoral Research Fellow — *Sep. 2003 - Mar. 2004*

- Quantum and quasi-classical calculations of rare gas with NO.
- Calculation of inelastic cross sections for OH–HCl system.
- Advisor: Prof. J. Aoiz

Institute of Theoretical Chemistry, University of Nijmegen — *Nijmegen, The Netherlands*

Postdoctoral Research Fellow — *Dec. 2001 - Aug. 2003*

- Developed quantum dynamics for F, Cl, Br-H_2 complexes.
- Calculation of bound states for Cl-HCl system.
- Advisor: A. van der Avoird

Teaching Experience

Department of Chemistry & Biochemistry, University of Maryland — *College Park, MD*

Course Instructor: Computational Chemistry CHEM-688C — *Spring 2016*

- 2-hour credit course for grad students: 1h lecture and 1h computational chemistry laboratory.
- Developed syllabus and course materials from scratch.
- Acquired necessary licenses and software for the course.
- Installed WebMO Pro server and linked remote computational engines to it.
- Installed Gaussian and GaussView on department lab computers.
- Used university's Canvas system for the course.

Department of Chemistry & Biochemistry, University of Maryland — *College Park, MD*

Teaching Associate: Physical Chemistry II CHEM-482 — *Spring 2010*

- Preparation of homework and exam's problem sets and solutions, selected lectures, office hours.
- Giving lectures during absence of the main lecturer.

Department of Chemistry & Biochemistry, University of Maryland — *College Park, MD*

Lecturer and Lab Instructor: Physical Chemistry Lab II CHEM-484 — *Fall 2006 & Spring 2007*

- 2-hour credit course: 1h lecture and 4h lab
- Preparation of Lab Manual.
- "round-robin" student groups in spectroscopy lab experiments, IR, UV/VIS etc.

Department of Chemistry, University of Warsaw — *Warsaw, Poland*

Teaching Assistant: Applications of Computers in Chemistry — *1997–2001*

- Topics on Molecular Modeling, database and citation search engines.
- Using MS Excel for regression and statistics of experimental measurements.

Department of Chemistry, University of Warsaw — *Warsaw, Poland*

Teaching Assistant: Quantum Chemistry course — *1997–2001*

- Fundamentals of quantum chemistry, solvable models of quantum mechanics, approximations in computational chemistry.

Visiting Academic Positions

Department of Chemistry, University of Le Havre — *Le Havre, France*

Visiting CNRS Professor — *Dec. 2014 - 1 Month*

- Program: Member of the Ph. D. thesis committee of Mario Hernandez, student of Prof. Francois Lique.

Department of Chemistry, Firat University — *Elazig, Turkey*

Visiting Professor — *Apr. 2014 - 1 Month*

- Program: Scientific collaboration with Prof. Niyazi Bulut within TUBITAK-112T827 grant.
- Performed installation and configuration of MPI libraries on Linux cluster for parallel time-dependent wavepacket calculations.

Department of Chemistry, University of Le Havre — *Le Havre, France*

Visiting Researcher — *Nov. 2009 - 10 days*

- Program: Scientific collaboration with Prof. Francois Lique in modeling of system of astrophysical interests.

Department of Chemistry, Complutense University — *Madrid, Spain*

Visiting Professor — *Feb. 2009 - 3 months*

- Program: Grant financed by Grupo-Santander "Seccion de Movilidad" for continuation of collaboration with spanish professors.
- Scientific collaboration with Prof. Javier Aoiz

Department of Chemistry, Universidad Autonoma del Estado de Morelos — *Cuernavaca, Mexico*

Visiting Researcher — *May 2007 - 2 weeks*

- Program: Collaboration with a group of Prof. Ramon Hernandez-Lamoneda under the support from the mexican Grant: CONACYT 44117E 2004-2008

Representative Publications

Publications in high-impact journals — *Science, Nature Chemistry*

- J. B. Kim, M. L. Weichman, T. F. Sjolander, D. M. Neumark, **J. Kłos**, M. H. Alexander, and D. E. Manolopoulos "Spectroscopic observation of resonances in the F+H_2 reaction" Science **349**, 510-513 (2015)
- E. Lavert-Ofir, Y. Shagam, A. B. Henson, S. Gersten, **J. Kłos**, P. S. Żuchowski, J. Narevicius, and E. Narevicius "Observation of the isotope effect in sub-kelvin reactions" Nature Chemistry **6**, 332 (2014)
- C. J. Eyles, M. Brouard, C.-H. Yang, **J. Kłos**, F. J. Aoiz, A. Gijsbertsen, A. E.Wiskerke, S. Stolte "Interference structures in the differential cross-sections for inelastic scattering of NO by Ar" Nature Chemistry **3**, 597-602 (2011)

Five most recent publications — *J. Chem. Phys., J. Phys. Chem. A, Phys. Rev. A*

- **J. Kłos**, M. H. Alexander, Q. Ma and P. Dagdigian "The interaction of NO($X^2\Pi$) with H_2: Ab initio potential energy surfaces and bound states" J. Chem. Phys. **146**, 114301 (2017)
- B. Jiang, P. Kumar, **J. Kłos**, M. H. Alexander, B. Poirier and H. Guo "First-principles C band absorption spectra of SO_2 and its isotopologues" J. Chem. Phys. **146**, 154305 (2017)
- P. Kumar, B. Jiang, H. Guo, **J. Kłos**, M. H. Alexander, and B. Poirier "Photoabsorption Assignments for the $\tilde{C}^1B_2 \leftarrow \tilde{X}^1A_1$ Vibronic Transitions of SO_2, Using New Ab Initio Potential Energy and Transition Dipole Surfaces" J. Phys. Chem. A **121** , 1012 (2017)
- **J. Kłos**, M. H. Alexander, P. Kumar, B. Poirier, B. Jiang and H. Guo "New *ab initio* adiabatic potential energy surfaces and bound state calculations for the singlet ground X and excited C states of SO_2" J. Chem. Phys. **144**, 174301 (2016)
- K. M. Hickson, J.-C. Loison, F. Lique, and **J. Kłos** "An Experimental and Theoretical Investigation of the $C(^1D) + N_2 \rightarrow C(^3P) + N_2$ Quenching Reaction at Low Temperature" J. Phys. Chem. A **120**, 2504 (2016)

Publications in Astrochemistry of Interstellar Media

Astr. J., A&A, MNRAS, PCCP

- S. Gómez-Carrasco, B. Godard, F. Lique, N. Bulut, **J. Kłos**, O. Roncero, A. Aguado, F. J. Aoiz, J. F. Castillo, J. R. Goicoechea, M. Etxaluze, and J. Cernicharo "OH^+ in astrophysical media: state-to-state formation rates, Einstein coefficients and inelastic collision rates with He" The Astrophysical Journal **794**, 33 (2014)
- M. Agúndez, J. Cernicharo, M. Guélin, C. Kahane, E. Roueff, **J. Kłos**, F. J. Aoiz, F. Lique, N. Marcelino, J. R. Goicoechea, M. González García, C. A. Gottlieb, M. C. McCarthy, and P. Thaddeus "Astronomical identification of CN^-, the smallest observed molecular anion" Astronomy & Astrophysics, **517**, L2, 1-5 (2010)
- M. Hernández Vera, F. Lique, F. Dumouchel, **J. Kłos**, J. Rubayo Soneira, and M.-L. Senent "Cyanide/isocyanide abundances in the interstellar medium - II. Inelastic rate coefficients of Al and Mg compounds" Mon. Not. R. Astron. Soc. **432**, 468 (2013)
- F. Lique, **J. Kłos** and M. Hochlaf "Benchmarks for the generation of interaction potentials for scattering calculations: Applications to rotationally inelastic collisions of $C_4(X^3\Sigma_g^-)$ with He" [Journal Issue Cover Art] Phys. Chem. Chem. Phys. **12**, 15672-15680 (2010)
- **J. Kłos** and F. Lique,"First rate coefficients for an interstellar anion: application to the $CN^{(-)}$–H_2 collisional system" Mon. Not. R. Astron. Soc. **418**, 271-275 (2011)
- M.-L. Dubernet, M. H. Alexander, Y. A. Ba, N. Balakrishnan, C. Balanćа, C. Ceccarelli, J. Cernicharo, F. Daniel, F. Dayou, M. Doronin, F. Dumouchel, A. Faure, N. Feautrier, D. R. Flower, A. Grosjean, P. Halvick, **J. Kłos**, F. Lique, G. C. McBane, S. Marinakis, N. Moreau, R. Moszynski, D. A. Neufeld, E. Roueff, P. Schilke, A. Spielfiedel, P. C. Stancil, T. Stoecklin, J. Tennyson, B. Yang, A.-M. Vasserot and L. Wiesenfeld "**BASECOL2012**: A collisional database repository and web service within the Virtual Atomic and Molecular Data Centre (VAMDC)" Astronomy & Astrophysics **553**, A50 (2013)

Cold Atoms and Molecules

J. Chem. Phys., PRA, PRL, PCCP

- J. J. Kay, **J. Kłos**, M. H. Alexander, K. E. Strecker and D. W. Chandler "Cold atoms by kinematic cooling" Phys. Rev. A, **82**, 032709 (2010)
- T. V. Tscherbul, T. A. Grinev, H.-G. Yu, A. Dalgarno, **J. Kłos**, Lifang Ma, and Millard H. Alexander "Cold collisions of polyatomic molecular radicals with S-state atoms in a magnetic field: An *ab initio* study of He + CH_2(X) collisions" J. Chem. Phys. **137**, 104302 (2012)
- M. T Hummon, T. V. Tscherbul, **J. Kłos**, Hsin-I Lu, E. Tsikata, W. C. Campbell, A. Dalgarno, and J. M. Doyle "Cold N+NH collisions in a magnetic trap" Phys. Rev. Lett. **106** 053201 (2011)
- Brian C. Sawyer, Benjamin K. Stuhl, Mark Yeo, Timur V. Tscherbul, Matthew T. Hummon, Yong Xia, **J. Kłos**, David Patterson, John M. Doyle, and Jun Ye "Cold heteromolecular dipolar collisions" Phys. Chem. Chem. Phys., **13** 19059 (2011)
- M. Kirste, L. Scharfenberg, **J. Kłos**, F. Lique, M. H. Alexander, G. Meijer, and S. Y. T. van de Meerakker "Low-energy inelastic collisions of OH radicals with He atoms and D_2 molecules" Phys. Rev. A, **82** 042717 (2010)

Simulations of chemical reactions

J. Chem. Phys., CPL, PCCP

- Mick Warehime, **J. Kłos**, and Millard H. Alexander "A finite-element visualization of quantum reactive scattering. II. Nonadiabaticity on coupled potential energy surfaces" J. Chem. Phys. **142**, 034108 (2015)
- A. Li, H. Guo, Z. Sun, **J. Kłos** and M. H. Alexander "State-to-state quantum dynamics of the F + HCl ($v = 0, j = 0$) $\rightarrow$ HF(v', j') + Cl reaction on the ground state potential energy surface" Phys. Chem. Chem. Phys. **15** 15347-15355 (2013)
- **J. Kłos**, P. Dagdigian and M. H. Alexander, "Theoretical study of the multiplet branching of the SD product in the $S(^1D)+D_2$ $\rightarrow SD(^2\Pi)+D(^2S)$ reaction" J. Chem. Phys., **127**, 154321 (2007)
- **J. Kłos**, Niyazi Bulut and Sinan Akpinar "Nonreactive scattering of the O^++H_2: A time-dependent wave packet approach" Chem. Phys. Lett. **532**, 22 (2012)
- **J. Kłos**, F. Lique, M. H. Alexander and P. J. Dagdigian "Theoretical determination of rate constants for vibrational relaxation and reaction of OH ($X^2\Pi$,v=1) with $O(^3P)$ atoms" J. Chem. Phys. **129**, 064306 (2008)

Inelastic scattering of radicals in the gas phase — *J. Chem. Phys., J. Phys. Chem. A, PCCP*

- H. C. Schewe, Q. Ma, N. Vanhaecke, X. Wang, **J. Kłos**, M. H. Alexander, S. Y. T. van de Meerakker, G. Meijer, A. van der Avoird, and P. J. Dagdigian "Rotationally inelastic scattering of OH by molecular hydrogen: Theory and experiment" J. Chem. Phys. **142**, 204310 (2015)
- S. Marinakis, I. L. Dean, **J. Kłos** and F. Lique "Collisional excitation of CH($X^2\Pi$) by He: new *ab initio* potential energy surfaces and scattering calculations" Phys. Chem. Chem. Phys. **17**, 21583 (2015)
- J. H. Lehman, M. I. Lester, **J. Kłos**, M. H. Alexander, P. J. Dagdigian, D. Herráez-Aguilar, F. J. Aoiz, M. Brouard, H. Chadwick, T. Perkins, and S. A. Seamons "Electronic Quenching of OH(A) Induced by Collisions with Kr Atoms" J. Phys. Chem. A **117**, 13481 (2013)
- **J. Kłos**, F. J. Aoiz, M. Menéndez, M. Brouard, H. Chadwick, and C. J. Eyles "*Ab Initio* studies of the interaction potential for the Xe-NO($X^2\Pi$) van der Waals complex: Bound states and fully quantum and quasi-classical scattering" J. Chem. Phys. **137**, 014312 (2012)
- J. D. Steill, J. J. Kay, G. Paterson, T. R. Sharples, **J. Kłos**, M. L. Costen, K. E. Strecker, K. G. McKendrick, M. H. Alexander, and D. W. Chandler "Rotational Alignment of NO ($A^2\Sigma^+$) from Collisions with Ne" J. Phys. Chem. A **117**, 8163 (2013)

Exhaustive list of publications — *See CV Appendix*

Citation Metrics

Web of Science

- Number of publications: 148
- Total number of citations: 2313
- H-index=26
- Average number of citations per article=17

Conference Presentations

Telluride Science Research Center (TSRC) Workshop — *Telluride, CO*

Invited Speaker — *Jun./5-10 2016*

- "New *ab initio* Potentials for the Ground and Excited Electronic States of SO_2 and SO"

Telluride Science Research Center (TSRC) Workshop — *Telluride, CO*

Invited Speaker — *Jan./11-15 2016*

- "Tailoring the Electronic Properties of Carbon Nanostructures"

XIII International Workshop on Quantum Reactive Scattering — *Salamanca, Spain*

Invited Speaker — *Jul./6-10 2015*

- "FEM in reactive scattering: Non-adiabatic scattering in F+HCl, F+H_2 and Li+CaH reactions"

XXVI International Symposium on Molecular Beams — *Segovia, Spain*

Poster — *Jun./28-Jul./3 2015*

- "Non-adiabatic reactive scattering with Finite Element Method:Application to F+HCl, F+H_2 and Li+CaH reactions"

Groupement de Recherche (GDR) Meeting — *University of Bordeaux, Bordeaux, France*

Invited Speaker — *Dec./9 2014*

- "Rotational Polarization over a Rainbow Theoretical and experimental studies of NO+Kr scattering"

Telluride Science Research Center (TSRC) Workshop *Telluride, CO*

Invited Speaker *Jan./12-16 2014*

- "Tests of *Ab Initio* Potentials in Chemical Dynamics of OH–H_2 and He*–H_2/HD/D_2 Systems"

Telluride Science Research Center (TSRC) Workshop *Telluride, CO*

Invited Speaker *Jul./15-19 2013*

- "Potentials and dynamics of complexes of NO and OH radicals in their excited states with noble gas atoms"

Quantum Lunch Series at Los Alamos National Laboratory *Los Alamos, NM*

Invited Seminar *Jul. 2013*

- Hosted by LANL employee Michael Di Rosa

Telluride Science Research Center (TSRC) Workshop *Silverton, CO*

Invited Speaker *Aug./9-13 2010*

- "OH in low energy collisions with noble gas, hydrogen, and ammonia"

Telluride Science Research Center (TSRC) Workshop *Telluride, CO*

Invited Speaker *Jan./7-11 2008*

- "Studies of electronic quenching of OH(A) in collisions with H_2: Theory versus Experiment"

Honors, Awards & Memberships

Honors & Awards

2002 **Prime Minister of Poland Award for best chemistry Ph. D. Thesis**, *Warsaw, Poland*

2002 **Foundation of Polish Academy of Science Award**, *Warsaw, Poland*

1992 **Finalist**, The Chemistry Olympiad *Warsaw, Poland*

Memberships

2016 **American Chemical Society**, *Regular member*

Skills

Networking CCNA, Cisco Networking Associate Course I, II and III, Routing and Switching, Scaling the Networks

Programming Fortran, Matlab, Python, Objective-C, Swift and Xcode environment, bash, csh

***Ab Initio* Codes** Molpro, Gaussian/GaussView, ADF, Gamess, Qchem

Scattering Codes Hibridon, Molscat, ABC, QCT-ABC

Typesetting and design LaTeX, MS Office, Adobe Illustrator

Educational systems and frontends Canvas, WebMO Pro

Operating Systems Linux, UNIX, Mac OS X, Windows

Compilers & Libraries Intel Fortran, Math Kernel Libraries, gfortran, Accelerate

Chemical Laboratory Glass work, IR and UV-VIS spectrometers, Gas Chromatography, titration e.t.c.

Work Permit

US Permanent Resident: since 2012

Professional References

- Upon request