CURRICULUM VITAE

Pavel A. Dub

Staff Scientist 3

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Education

Ph.D.	Organometallic Chemistry, Université de Toulouse & CNRS, France, 2010 *Supervisor:* Professor Rinaldo Poli *Thesis title*: Platinum-catalyzed hydroamination of ethylene: experimental and theoretical studies and its mechanism
Ph.D.	Physical Chemistry, A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Russia, 2009 *Supervisor:* Professor Elena S. Shubina *Thesis title*: Influence of the nature of the metal atom, the ligand environment, and the nature of the solvent on the mechanism of protonation of Cp* hydride complexes of Mo and metals of the Iron subgroup
M.S.	Higher Chemical College, Russian Academy of Sciences, Russia, 2007 (*summa cum laude*)

Employment Experience

2019	Project Lead, "Quantum Chemistry on Quantum Computers" (4.8M$, FY 2020-2023). Leading the team of 19 staff scientists & postdocs & students focused on the development of algorithms to solve quantum chemistry problems on near-term gate-based quantum computers and quantum annealers. Got the team to deliver successful project with large number of products long before the milestones. Initiated first-ever quantum chemistry simulations on NISQ quantum architectures at LANL. LANL representative for quantum chemistry calculations on NISQ.
2016-	Staff Scientist 3, Chemistry Division, Los Alamos National Laboratory, NM, USA Mentoring and leading research in the field of organometallic & inorganic chemistry, applied homogeneous (asymmetric) catalysis with (chiral) molecular complexes, computational homogeneous catalysis on High-Performance CPU/GPU architectures (static and dynamic DFT methods).
2013-2016	J. Robert Oppenheimer Distinguished Postdoctoral Fellow, Los Alamos National Laboratory, NM, USA. Development of ligands and catalysts for practical hydrogenation of biorenewable esters
2010-2013	JSPS Postdoctoral Fellow, Tokyo Institute of Technology, Japan *Supervisor:* Professor Takao Ikariya. Rational design of new bifunctional catalysis.

Selected Awards and Recognitions

2020	STREM Chemicals Inc. commercialized Dub Homogeneous Ruthenium Catalysts for Ester Hydrogenations
2018	A molecular Ir catalyst developed by Pavel Dub of Chemistry Division at LANL was featured in a cover image of the latest issue of *Nature Reviews Chemistry* (2018, volume 2, issue 12). The catalyst is commercially available from STREM CHEMICAL, INC.
2018	2018 Publons Peer Review Award (Top 1% Peer-Reviewer in Chemistry)
2017	Book "Enantioselection in Asymmetric Catalysis" highlighted by Prof. Tsuneo Imamoto in the *Journal of Tokyo Chemical Industry Co*., Ltd. # TCIMAIL 174.

2014 Los Alamos National Laboratory J. Robert Oppenheimer (JRO) Distinguished Postdoctoral Fellowship (one of 2 appointments per year, open to all nationalities, typically around 1000 applicants for postdoctoral positions/yr. "Candidates for LANL Distinguished Postdoctoral Fellows display extraordinary ability in scientific research and show clear and definite promise of becoming outstanding leaders in the research they pursue").

2010 JSPS (Japan Society for the Promotion of Science) Postdoctoral Research Fellowship 2010-2012 (1168 applications were received in FY 2010–2011, among which 150 fellowships were awarded); Grant-in-Aid for Scientific Research for JSPS Postdoctoral Research Fellows.

Major Research Interests

Experimental (wet) Chemistry → organometallic & inorganic chemistry (synthesis & isolation and characterization), physical chemistry and kinetics, applied homogeneous (asymmetric) catalysis with (chiral) molecular complexes (design, process development, scale-up), catalyst commercialization, patent development, molecular spectroscopy (NMR, EPR, IR, UV) .

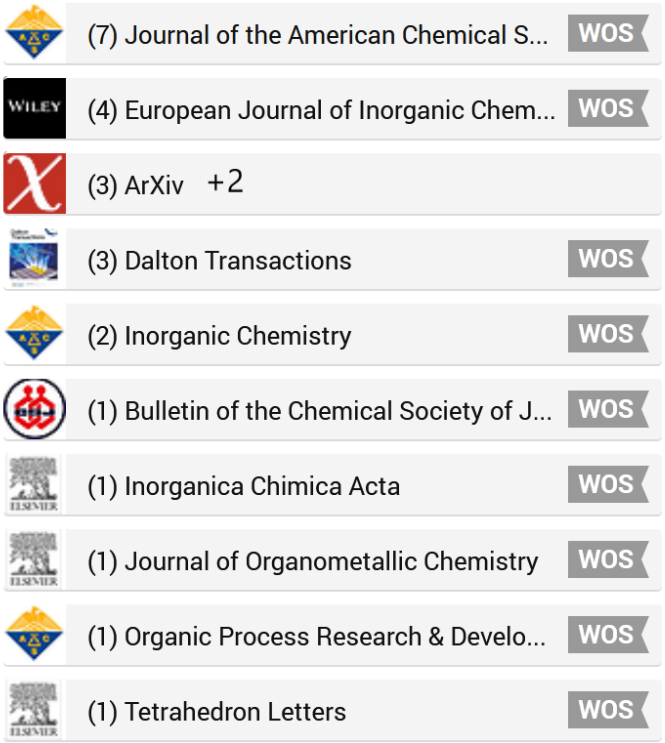
Computational & Quantum Chemistry → electronic structure, computational homogeneous catalysis on High-Performance CPU/GPU architectures (static and dynamic DFT methods, e.g. ab initio molecular dynamics), reaction mechanisms, quantum information science, Python programming, quantum computing, simulations on IBM Q and D-WAVE, electronic structure of molecules on near-term gate-based quantum computers and quantum annealers.

Research Funding (since at Los Alamos National Laboratory, 2013-current) $22.9M ($5.7M as PI)

Year	Source (PI=Principal Investigator, coINV=co-investigator)	Amount
2021	DOE BES 2022–2025 "Molecular complexation of rare earth elements (REE) in high temperature and pressure supercritical geologic fluids" (coINV; PI: Alexander Gysi, New Mexico Tech)	$2.7M
2021	DOE BES 2022–2025 "Data science driven quantum chemistry for reactive chemistry controlled by stimuli" (coINV; PI: Kipton Barros, LANL; co-PI: Garnet Chen, Caltech)	$2.4M
2021	LANL LDRD DR 2022–2025 20210073DR "Scalable Molecular Framework Architectures for Qubit Control and State Transduction" (coINV; PI: Jennifer Hollingsworth, LANL)	$5.1M
2021	LANL LDRD DR 2022–2025 20220053DR "Accelerating Nuclear Fuel Qualification through Integrated Multiscale and Multiphysics Models" (coINV; PI: Tammie Nelson, LANL)	$5.1M
2020	LANL LDRD DI 20210737DI "Data Driven Accelerated Fuel Qualification for Nuclear Fuels" (coINV; PI: Tammie Nelson, LANL)	$0.7M
2019	LANL LDRD DR 2020–2023 20200056DR "Quantum Chemistry on Quantum Computers" (PI)	$4.8M
2019	DOE BES 2020–2023 CX-101636 "Hydrogen Release from Concentrated Media with Reusable Catalysts" (coINV; PI: Travis Williams, USC)	$1.25M
2018	LANL LDRD Reserve Fund 2019 20190607ER "Variational Quantum Eigensolver for H_2O" (PI)	$0.15M
2016	LANL LDRD Reserve Fund 2016 20160666ER "New Ligands and Catalysts for the Hydrogenation of Renewable Compounds Containing Ester Functionality" (PI)	$0.10M
2014	LANL LDRD J. Robert Oppenheimer Distinguished Postdoctoral Fellowship 2014–2017 20140672PRD2 "Access to Industrially Important Optically Active beta-X-alcohols via Direct Enantioselective Ester Hydrogenation" (PI)	$0.63M

Life-time Count of Research Productivity (2005-current)

- Books	1	- Review articles	4
- Patents	3	- Nature-family journals	4+1*
- Papers in refereed journals	47+5*	- Invited contributions	4
- ArXiv	5	- Corresponding/last author	23
- First Author	33		



*Submitted: *npj Quantum Information*, *Quantum Inf. Process*, *Sci. Rep.*, *Plos One*, *J. Chem. Inf. Model*

ORCID ID: 0000-0001-9750-6603, h-index: 22, ~2000 citations (Google Scholar)

Invited and Selected Oral Talks

EuCOMC 2021, Madrid, Spain (invited keynote speaker).**
International Conference on Chemical Bonding (Organizers: A. Boldyrev, A. Alexandrova, L.-S. Wang), postponed to 2022, Kauai, HI, USA (invited).**
The Cutting-Edge Homogeneous Catalysis International Workshop-1 (CEHC-1, on-line event), May 4-6, 2021, Toulouse, France.
PNNL (host: R. Morris Bullock), August 7th, 2019, Richland, WA, USA (invited).
ZIOC RAS (Ananikov Lab), July 26th, 2018, Moscow, Russia (invited).
2018 ACS Meeting in New Orleans, LA, March 18–22, 2018.
2017 Gordon Research Conference (GRC) on Organometallic Chemistry in Newport, RI, July 9–14, 2017 (short talk selected from poster session).
2017 ACS Meeting in San Francisco, CA, April 2–6, 2017.
2016 Gordon Research Conference (GRC) on Green Chemistry in Stowe, VT, July 31 - August 5, 2016 (short talk selected from poster session);
2016 ACS Meeting in San Diego, CA, March 13–17, 2016 (invited, Symposium in honor of Richard Martin).
Pacifichem 2015 in Honolulu, HI, December 15–20, 2015 (invited).
The 93rd Annual Meeting of CSJ in Kyoto, March 22–17, 2013, Japan.
**postponed to 2022

Service

> 90 journal peer-reviews, 3 large-scale grant reviews in 2021
Publons: publons.com/a/1308714/

Proposals reviewed in **2021**

- The Office of Basic Energy Sciences (BES) within the Department of Energy (DOE) Office; DE-FOA-0002441, Scientific Discovery Through Advanced Computing (SciDAC): Partnerships in Basic Energy Sciences (two proposals reviewed, total funding 8M$ each)
- French National Research Agency (ANR) 2021 (AAPG2021) “Chimie moléculaire” evaluation panel (total funding 437 k€).
- LANL LDRD ER Computational Methods and Computer Science (CMCS) Technical Category evaluation panel (5 proposals selected, total funding 4.8M$)

Teaching/Mentorship experience

Instructor: Supervision of Masters level chemistry students at Tokyo Institute of Technology; trainees from the Lycée Jolimont, France; 1st year students from the Higher Chemical College RAS (coursework in inorganic chemistry), Russia.

Teaching Assistant: Travaux Dirigés de Thermodynamique Chimique (L1, seconde semester, 2010), Université Paul Sabatier, Toulouse, France (class, ~30 students).

Notable former students/postdocs mentored: Dr. Alexander Teplukhin (Ph.D. with Prof. Dmitri Babikov, Marquette University); Postdoctoral Research Associate. Topic: Quantum Annealer Eigensolver; Dr. Asuka Matsunami (Ph.D. with Prof. Takao Ikariya, TokyoTech, Japan), Assistant Professor, Department of Chemistry and Biological Science, Aoyama Gakuin University, Tokyo, Japan; Dr. Gleb Silantyev (Ph.D. with Prof. Natalia Belkova, INEOS RAS, Russia), Postdoc with Prof. S. Schneider, Georg-August-Universität Göttingen, Germany; current position: CAT Catalytic Center Aachen, Germany.

Current postdocs/students mentored/co-mentored at LANL: Dr. Ashutosh Kumar, (Ph.D. with Prof. T. Daniel Crawford, Virginia Tech); Postdoctoral Research Associate. Topic: Excited States Algorithms Implementation on Gate-based Quantum Computers; Dr. Rami Batrice, (Ph.D. with Prof. Moris Eisen, The Technion, Israel); Director’s Postdoctoral Fellow. Topic: Engineering Homogeneous Catalysts for Biorenewable Ester Hydrogenation; Nikolay Tkachenko, (Ph.D. candidate with Prof. Alexander Boldyrev, Utah State), summer 2020 & 2021 student. Topic: Quantum Davidson Algorithm; James Sud, (Quantum Programmer at Berkeley Lab, University of California, Berkeley), LANL summer 2020 Quantum School. Topic: Permutation Variational Quantum Eigensolver; Diana Chamaki (UC Berkeley Physics), LANL summer 2021 Quantum School. Topic: Non-adiabatic Molecular Dynamics on Quantum Computers; Dewi Yokelson (University of Oregon Computer Science), LANL summer 2021 HPC School. Topic: Performance Analysis of CP2K Code for Ab Initio Molecular Dynamics for Homogeneous Catalysis.

Profiles

: https://www.linkedin.com/in/pavel-a-dub-a90a3385
: https://www.researchgate.net/profile/Pavel-Dub
: publons.com/a/1308714/
: https://scholar.google.com/citations?user=4yvZG2AAAAAJ&hl=en

Selected Scientific Production

STREM (selected commercialized molecular catalysts developed by PAD):
Ru: https://www.strem.com/catalog/v/44-3210/59/ruthenium_1802182-33-7
Ir: https://www.strem.com/catalog/v/77-0560/31/iridium_1839552-43-0

(book): https://www.amazon.com/Enantioselection-Asymmetric-Catalysis-4x45-Gridnev/dp/1498726542

REFERENCES

Names and Email Addresses

Pavel A. Dub, PH.D. Staff
Scientist 3, LANL

1. **Dr. R. Morris Bullock**

   Pacific Northwest National Laboratory, Richmond,
   WA, USA Email: morris.bullock@pnnl.gov

2. **Professor Rinaldo Poli**
   ENSIACET and Laboratoire de Chimie de
   Coordination UPR CNRS 8241, Toulouse, France
   Email: Rinaldo.Poli@lcc-toulouse.fr

3. **Professor Johannes G. de Vries**
   Leibniz-Institut für Katalyse, Rostock, Germany
   Email: Johannes G. de Vries
   Johannes.deVries@catalysis.de

4. **Professor Sergei Tretiak**
   Los Alamos National Laboratory, Los Alamos, NM,
   USA Email: serg@lanl.gov

Publication List

Pavel A. Dub

Los Alamos National Laboratory

h-index: 22, ~2000 citations (Google Scholar)
Experimental Organometallic Chemistry & Homogeneous Catalysis papers are highlighted
Computational Homogeneous Catalysis on HPC papers are highlighted
Quantum Chemistry & Computing papers are highlighted

Publications (since at Los Alamos National Laboratory, * = PI and corresponding author)

In Preparation for Submission in 2022

57. Zhang, G.*; **Dub, P. A.*** Markovnikov Alcohols via Epoxide Hydroboration with Catalytic Amount of Super Hydride *J. Am. Chem. Soc.* 2022 (in preparation)
56. Negre, C.F.A.*; Lopez-Bezanilla, A.; Zhang, Y.; Akrobotu, P.; Mniszewski, S. M; Tretiak, S.; **Dub, P. A.** QUBO-based density matrix electronic structure method. *J. Chem. Theory Comput*. 2022 (in preparation)
55. Schleich, P.; Zhang, Y.; Cincio, L.*; Coles, P. J.; Tretiak, S.; **Dub, P. A.** Quantum Chemistry with Near-Clifford Circuits. *Npj Quantum Information* 2022 (in preparation)
54. Chamaki, D.; Bultrini, D.; Tkachenko, N. V.; Zhang, Y.*; Cincio, L.; Coles, P. J.; Boldyrev, A.; Tretiak, S.; **Dub, P. A.*** Non-adiabatic molecular dynamics on quantum computers. *J. Chem. Theory Comput*. 2022 (in preparation)
53. Tkachenko, N. V.; Zhang, Y.*; Cincio, L.; Coles, P. J.; Boldyrev, A.; Tretiak, S.; **Dub, P. A.*** Quantum Davidson algorithm for Excited States. *PRX Quantum* 2022 (in preparation)

Submitted

52. Gayday, I.; Babikov, D.*; Teplukhin, A.; Kendrick, B. K.; Mniszewski, S. M.; Zhang, Y.; Tretiak, S.; **Dub, P. A.*** Molecular Dynamics on Quantum Annealers. *Sci. Rep.* 2022 (submitted, arXiv:2110.12096).
51. Yokelson, D.; Tkachenko, N. V.; Robey, R.; Li, Y.-W.; **Dub, P. A.*** Performance Analysis of CP2K Code for Ab Initio Molecular Dynamics on CPUs and GPUs. *J. Chem. Inf. Model.* 2022 (submitted, arXiv:2109.04536).
50. Gu, A.; Lowe, A.; **Dub, P. A.**; Coles, P. J.; Arrasmith, A.* Adaptive shot allocation for fast convergence in variational quantum algorithms. *Quantum Sci. Technol*. 2022 (submitted, arXiv:2108.10434).
49. Zhang, Y.*; Cincio, L.; Negre, CFA; Czarnik, P.; Coles, P. J.; Mniszewski, S. M.; Anisimov, P.; Tretiak, S.; **Dub, P. A.**, Variational Quantum Eigensolver with Reduced Circuit Complexity. *Npj Quantum Inf.* 2022 (under review, arXiv:2106.07619).
48. Teplukhin, A.; Kendrick, B. K*.; Mniszewski, S. M.; Tretiak, S.; **Dub, P. A.**,* Sampling electronic structure QUBOs with Ocean and Mukai solvers. *Plos One* 2022 (under review, arXiv:2102.01225).

Published

2021

47. **Dub, P. A**.* Alkali Metal Alkoxides in Noyori-type Hydrogenations (A Celebratory Collection in EurJIC for Professor Rinaldo Poli). *Eur. J. Inorg. Chem.* 2021, 4884–4889. *Selected as Very Important Paper (VIP).*

46. Teplukhin, A.; Kendrick, B. K.; Mniszewski, S. M.; Zhang, Y.; Kumar, A.; Negre, CFA; Anisimov, P.; Tretiak, S.*; **Dub, P. A.***, Computing molecular excited states on a D-Wave quantum annealer. *Sci. Rep.* 2021, 11, 18796.
45. **Dub, P. A.***; Tkachenko, N. V., Mechanism of Potassium tert-Butoxide–Catalyzed Ketones Hydrogenation in Solution-Phase (The Journal of Physical Chemistry virtual special issue "Alexander Boldyrev Festschrift"). *J. Phys. Chem. A*, 2021, 125, 26, 5726–5737.
44. **Dub, P. A.***; Tkachenko, N. V.; Vijesh, V.; Wills, M.; Smith, J. S.; Tretiak, S., Enantioselectivity in the Noyori–Ikariya Asymmetric Transfer Hydrogenation of Ketones. *Organometallics* 2021, 40 (9), 1402–1410.
43. Tkachenko, N. V.; Sud, J.; Zhang, Y.*; Tretiak, S.; Anisimov, P. M.; Arrasmith, A. T.; Coles, P. J.; Cincio, L.*; **Dub, P. A.***, Correlation-informed permutation of qubits for reducing ansatz depth in the Variational Quantum Eigensolver. *PRX Quantum* 2021, 2, 020337.
42. Mniszewski, S. M.; **Dub, P. A.**; Tretiak, S.; Anisimov, P. M.; Zhang, Y.; Negre, C. F. A., Reduction of the molecular hamiltonian matrix using quantum community detection. *Sci. Rep.* 2021, 11 (1), 4099.

2020

41. Teplukhin, A.; Kendrick, B. K.*; Tretiak, S.; **Dub, P. A.***, Electronic structure with direct diagonalization on a D-wave quantum annealer. *Sci. Rep*. 2020, 10 (1), 20753.
40. **Dub, P. A.***; Batrice, R. J.; Gordon, J. C.; Scott, B. L.; Minko, Y.; Schmidt, J. G.; Williams, R. F., Engineering Catalysts for Selective Ester Hydrogenation. *Org. Process Res. Dev.* 2020, *24* (3), 415-442.

2019

39. **Dub, P. A.***; Batrice, R. J.; Gordon, J. C. Synthesis of fluoral hemiacetals and hemiaminals via transition metal-catalyzed ester hydrogenation. WO2015191505A1, 2019.
38. Zhang, G.*; Wu, J.; Zheng, S.; Neary, M. C.; Mao, J.; Flores, M.; Trovitch, R. J.; **Dub, P. A.***, Redox-Noninnocent Ligand-Supported Vanadium Catalysts for the Chemoselective Reduction of C=X (X = O, N) Functionalities. *J. Am. Chem. Soc.* 2019, *141* (38), 15230-15239.
37. Zhang, G.*; Wu, J.; Zeng, H.; Neary, M. C.; Devany, M.; Zheng, S.; **Dub, P. A.***, Dearomatization and Functionalization of Terpyridine Ligands Leading to Unprecedented Zwitterionic Meisenheimer Aluminum Complexes and Their Use in Catalytic Hydroboration. *ACS Catal.* 2019, *9* (2), 874-884.

Publications (at Los Alamos National Laboratory – Postdoctoral work)

2018

36. **Dub, P. A.***; Gordon, J. C.*, The role of the metal-bound N-H functionality in Noyori-type molecular catalysts. *Nat. Rev. Chem.* 2018, *2* (12), 396-408.

2017

35. **Dub, P. A.***; Scott, B. L.; Gordon, J. C.*, Why Does Alkylation of the N-H Functionality within M/NH Bifunctional Noyori-Type Catalysts Lead to Turnover? *J. Am. Chem. Soc.* 2017, *139* (3), 1245-1260.
34. **Dub, P. A.***; Gordon, J. C.; Schmidt, J. G.; Minko, Y.; Williams, R. F. Macrocyclic ligands and their complexes for bifunctional molecular catalysis. Patent number: 10487100 (Application Number: 15/944,503), 2017.
33. **Dub, P. A.***; Gordon, J. C., Metal-Ligand Bifunctional Catalysis: The "Accepted"

Mechanism, the Issue of Concertedness, and the Function of the Ligand in Catalytic Cycles Involving Hydrogen Atoms. *ACS Catal.* 2017, *7* (10), 6635-6655.

32. Gridnev, I. D.*; **Dub, P. A.***, *Enantioselection in Asymmetric Catalysis*. CRC Press (Taylor Francis): 2016/17.

2016

31. **Dub, P. A.***; Scott, B. L.; Gordon, J. C.*, First-row transition metal complexes of ENENES ligands: the ability of the thioether donor to impact the coordination chemistry. *Dalton Trans.* 2016, *45* (4), 1560-1571.
30. **Dub, P. A.***; Gordon, J. C.*, The mechanism of enantioselective ketone reduction with Noyori and Noyori-Ikariya bifunctional catalysts. *Dalton Trans.* 2016, *45* (16), 6756-6781.

2015

29. **Dub, P. A.***; Gordon, J. C. Polydentate ligands and their complexes for molecular catalysis. US20170088571A1, 2015.
28. **Dub, P. A.***; Scott, B. L.; Gordon, J. C.*, Air-stable NNS (ENENES) ligands and their well-defined ruthenium and iridium complexes for molecular catalysis. *Organometallics* 2015, *34* (18), 4464-4479.

2014

27. **Dub, P. A.***; Henson, N. J.; Martin, R. L.; Gordon, J. C.*, Unravelling the Mechanism of the Asymmetric Hydrogenation of Acetophenone by [RuX_2(diphosphine)(1,2-diamine)] Catalysts. *J. Am. Chem. Soc.* 2014, *136* (9), 3505-3521.

Publications (at Tokyo Institute of Technology – Postdoctoral work)

2019

26. **Dub, P. A.***; Matsunami, A.; Kuwata, S.; Kayaki, Y.*, Cleavage of N–H Bond of Ammonia via Metal-Ligand Cooperation Enables Rational Design of a Conceptually New Noyori-Ikariya Catalyst. *J. Am. Chem. Soc.* 2019, *141* (6), 2661-2677.

2013

25. **Dub, P. A.**; Wang, H.; Matsunami, A.; Gridnev, I. D.; Kuwata, S.; Ikariya, T.*, C-F bond breaking through aromatic nucleophilic substitution with a hydroxo ligand mediated via water bifunctional activation. *Bull. Chem. Soc. Jpn.* 2013, *86* (5), 557-568.
24. **Dub, P. A.**; Ikariya, T.*, Quantum Chemical Calculations with the Inclusion of Nonspecific and Specific Solvation: Asymmetric Transfer Hydrogenation with Bifunctional Ruthenium Catalysts. *J. Am. Chem. Soc.* 2013, *135* (7), 2604-2619.
23. Otsuka, T.; Ishii, A.; **Dub, P. A.**; Ikariya, T.*, Practical Selective Hydrogenation of α-Fluorinated Esters with Bifunctional Pincer-Type Ruthenium(II) Catalysts Leading to Fluorinated Alcohols or Fluoral Hemiacetals. *J. Am. Chem. Soc*. 2013, 135 (26), 9600-9603.

2012

22. **Dub, P. A.**; Wang, H.; Watanabe, M.; Gridnev, I. D.; Ikariya, T.*, A practical asymmetric conjugate addition to cyclic enones with chiral bifunctional Ru amido catalysts. *Tetrahedron Lett.* 2012, *53* (27), 3452-3455.
21. **Dub, P. A.**; Ikariya, T.*, Catalytic Reductive Transformations of Carboxylic and Carbonic Acid Derivatives Using Molecular Hydrogen. *ACS Catal.* 2012, *2* (8), 1718-1741.

Publications (at Laboratoire de Chimie de Coordination UPR CNRS – Ph.D. work)

2013

20. Bethegnies, A.; **Dub, P. A.**; Poli, R.*, Platinum-catalyzed assembly of quinaldine from

aniline and ethylene. *Organometallics* 2013, 32 (6), 1882-1891.

2012

19. **Dub, P. A.**; Bethegnies, A.; Daran, J.-C.; Poli, R.*, Formation and Structure of a Platinum(II) Complex Containing Two trans Nonstabilized Phosphorus Ylide Ligands: Evidence for Reversible Ylide Dissociation. *Organometallics* 2012, *31* (8), 3081-3086.
18. **Dub, P. A.**; Bethegnies, A.; Poli, R.*, DFT and experimental studies on the PtX_2/X^--catalyzed olefin hydroamination: effect of halogen, amine basicity, and olefin on activity, regioselectivity, and catalyst deactivation. *Organometallics* 2012, *31* (1), 294-305.

2011

17. **Dub, P. A.**; Bethegnies, A.; Poli, R.*, Reactions of diethylamine and ethylene catalyzed by PtII or Pt0 - Transalkylation vs. Hydroamination. *Eur. J. Inorg. Chem.* 2011, *2011* (33), 5167-5172.
16. **Dub, P. A.**; Daran, J.-C.; Levina, V. A.; Belkova, N. V.; Shubina, E. S.; Poli, R.*, Modeling the platinum-catalyzed intermolecular hydroamination of ethylene: The nucleophilic addition of $HNEt_2$ to coordinated ethylene in *trans*-PtBr2(C2H4)(HNEt2). *J. Organomet. Chem.* 2011, *696* (6), 1174-1183.

2010

15. **Dub, P. A.**; Rodriguez-Zubiri, M.; Baudequin, C.; Poli, R.*, Hydroamination of ethylene by aniline: catalysis in water. *Green Chem.* 2010, *12* (8), 1392-1396.
14. **Dub, P. A.**; Poli, R.*, The Pt-catalyzed ethylene hydroamination by aniline: a computational investigation of the catalytic cycle. *J. Am. Chem. Soc.* 2010, *132* (39), 13799-13812.
13. **Dub, P. A.**; Poli, R.*, A computational study of solution equilibria of platinum-based ethylene hydroamination catalytic species including solvation and counterion effects: Proper treatment of the free energy of solvation. *J. Mol. Catal. A: Chem.* 2010, *324* (1-2), 89-96.

2009

12. **Dub, P. A.**; Filippov, O. A.; Belkova, N. V.; Rodriguez-Zubiri, M.; Poli, R.*, Experimental (IR, Raman) and Computational Analysis of a Series of $PtBr_2$ Derivatives: Vibrational Coupling in the Coordinated Ethylene and Pt-Br Modes. *J. Phys. Chem. A* 2009, *113* (22), 6348-6355.
11. **Dub, P. A.**; Rodriguez-Zubiri, M.; Daran, J.-C.; Brunet, J.-J.; Poli, R.*, Platinum-Catalyzed Ethylene Hydroamination with Aniline: Synthesis, Characterization, and Studies of Intermediates. *Organometallics* 2009, *28* (16), 4764-4777.

Publications (at A. N. Nesmeyanov Institute of Organoelement Compounds – Ph.D. and M.S. works)

2010

10. **Dub, P. A.**; Belkova, N. V.; Filippov, O. A.; Daran, J.-C.; Epstein, L. M.; Lledos, A.; Shubina, E. S.; Poli, R.*, Solvent-Dependent Dihydrogen/Dihydride Stability for $[Mo(CO)(Cp^*)H_2(PMe_3)_2]^+[BF_4]^-$ Determined by Multiple Solvent···Anion···Cation Non-Covalent Interactions. *Chem. - Eur. J.* 2010, *16* (1), 189-201, S189/1-S189/35.
9. **Dub, P. A.**; Filippov, O. A.; Belkova, N. V.; Daran, J.-C.; Epstein, L. M.; Poli, R.; Shubina, E. S.*, Hydrogen bonding to carbonyl hydride complex $Cp^*Mo(PMe_3)_2(CO)H$ and its role in proton transfer. *Dalton Trans.* 2010, *39* (8), 2008-2015.
8. **Dub, P. A.**; Fillipov, O. A.; Silantyev, G. A.; Belkova, N. V.; Daran, J.-C.; Epstein, L. M.; Poli, R.; Shubina, E. S.*, Protonation of Cp*M(dppe)H Hydrides: Peculiarities of the Osmium Congener. *Eur. J. Inorg. Chem.* 2010, (10), 1489-1500.

2009

7. Baya, M.; **Dub, P. A.**; Houghton, J.; Daran, J.-C.; Belkova, N. V.; Shubina, E. S.*; Epstein,

L. M.; Lledos, A.; Poli, R.*, Investigation of the $[Cp^*Mo(PMe_3)_3H]^{n+}$ (n = 0, 1) Redox Pair: Dynamic Processes on Very Different Time Scales. *Inorg. Chem.* 2009, *48* (1), 209-220.

2008

6. **Dub, P. A.**; Belkova, N. V.; Lyssenko, K. A.; Silantyev, G. A.; Epstein, L. M.; Shubina, E. S.*; Daran, J.-C.; Poli, R.*, Synthesis and Protonation Studies of Cp*Os(dppe)H: Kinetic versus Thermodynamic Control. *Organometallics* 2008, *27* (13), 3307-3311.

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