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⋆ 1980	Przemyslaw Dopieralski
1999–2004	Studies of Chemistry at Univeristy of Wroclaw, Poland Faculty of Chemistry
2004	Diplom in Chemistry, Univeristy of Wroclaw, Poland Faculty of Chemistry (Prof. Zdzislaw Latajka) *Theoretical modelling of nonlinear electrooptical properties of HF with nitropyridines*
2004–2008	PhD studies at Univeristy of Wroclaw, Poland Faculty of Chemistry (Prof. Zdzislaw Latajka)
2006	Visiting Scientist at Ruhr Universität Bochum, Germany Lehrstuhl für Theoretiche Chemie (Prof. Dominik Marx) *Path Integrals Molecular Dynamics*
2008	PhD at Univeristy of Wroclaw, Poland Faculty of Chemistry (Prof. Zdzislaw Latajka) *Theoretical study on proton motion in dicarboxylic acids crystals by Car-Parrinello molecular dynamics*
2009–2013	Posdoctoral Fellow at Ruhr Universität Bochum, Germany Lehrstuhl für Theoretiche Chemie (Prof. Dominik Marx) *Mechanochemistry*
2013 – now	Adjunct – Univeristy of Wroclaw, Poland Faculty of Chemistry

Contact

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Personal details

Birthday:	1.11.1980, Świdnica, Poland
Marital status:	married, dr. Sylwia Dopieralska (Pilorz), 20.10.2007
Kids:	Adam Aleksander Dopieralski, 18.07.2009
	Dominik Adam Dopieralski, 23.03.2012

Computer skills

	poor	○ ○ ○ ○ ○
	excellent	● ● ● ● ●
HPC	IBM platform - BlueGene/P/Q	● ● ● ● ●
Operating SYS.	Linux, Windows	● ● ● ● ●
MS Office	Word, Excell, PowerPoint, Access	● ● ● ● ○
Computer lang.	Fortran, C++, Prolog, TurboPascal	● ● ● ● ○
	awk	● ● ● ● ○
	Mathlab	● ● ● ○ ○
	LaTeX	● ● ● ● ●
Chemistry soft.	Car-Parrinello Molecular Dynamics	● ● ● ● ●
	Path Integrals Molecular Dynamics	● ● ● ● ●
	Gaussian, TurboMole, Gamess	● ● ● ● ●
	Omnic, Grams	● ● ● ○ ○
	VMD, Molden, Molekel, Mercury	● ● ● ● ○
	GaussView	● ● ● ● ○
Other	CorelDraw, Gimp, xmgrace	● ● ● ● ○

Other skills

Series of presentations: Kyiv (Ukraine,2006), Trieste (Italy,2008,2011), St. Petersburg (Russia,2007), Barcelona (Spain,2011), Budapest (Hungary, 2013)
Series of lectures on: Quantum Chemistry, Chemical calculations, molecular modeling (english and polish)
Course of Information Technology in management (2004)
Driving license (1997)

learning abilities	●●●●●
teaching	●●●●●
creativeness	●●●●●
resistance to stress	●●●●●

Languages

polish (native)	●●●●●
english (FCE)	●●●●○
german	●●○○○

2011–2017 Jülich BlueGene/Q
Mechanochemistry of Covalent Bond Breaking from First Principles Simulations
- project manager

2014–now Member of the *Academy of Young Scholars and Artists*

Teaching and other employment

2009–2017 Erasmus Mundus Course of Molecular Design of New Materials (in English)
Faculty of Chemistry, University of Wroclaw
14, F. Joliot-Curie Str.
50-383 Wroclaw, Poland

2008–2009 IT teacher at Privat High School EKOLA (in English)
56, T. Zielinskiego Str.
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References

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Group Home Page

Professor Dr. hab. Zdzislaw Latajka
Head of the Theoretical Modeling of Chemical Processes Group
Full Professor, Senior Lecturer
Faculty of Chemistry, University of Wroclaw
14, F. Joliot-Curie Str.
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Professor Dr. Dominik Marx
Lehrstuhl für Theoretische Chemie
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D-44780 Bochum
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Home Page

Invited Reviews, Features, and Lecture Notes

4. P. Dopieralski, Z. Latajka
"Computational mechanochemistry." in "Practical aspects of computational chemistry IV",
2016, 233-243. ISBN 978-1-4899-7697-0

3. P. Dopieralski, J. Ribas–Arino, D. Marx
Force-activated Reactivity of Disulfides or the "Strange case of Dr. Jekyll and Mr. Hyde"
John von Neumann Institute for Computing (NIC) Julich 2014, vol 47, pp. 131-138
Eds. K. Binder, G. Munster, R. Kremer

2. P. Dopieralski, J. Ribas–Arino, D. Marx
Mechanochemistry of Covalent Bond Breaking from First Principles Simulations
John von Neumann Institute for Computing (NIC) Julich 2012, vol 45, pp. 115-122
Eds. K. Binder, G. Munster, R. Kremer

1. P. Dopieralski, P. Anjukandi, J. Ribas–Arino, D. Marx
Theoretical Mechanochemistry: Stressing Molecules in the Virtual Lab
InSiDE (Innovatives Supercomputing in Deutschland) 2012, vol. 10, pp. 48-52

List of publications

19. M. Krupicka, P. Dopieralski, D. Marx
Unclicking the Click: Metal–assisted Mechanochemical Cycloreversion of Triazoles is Possible
Angew. Chem. Int. Ed. 56, 7745–7749 (**2017**) doi:10.1002/anie.201612507
ImpF: **11.3**

18. P. Dopieralski, J. Ribas–Arino, P. Anjukandi, M. Krupicka, D. Marx
Unexpected mechanochemical complexity in the mechanistic scenarios of disulfide bond reduction
Nat. Chem. 9, 164–170 (**2017**) doi:10.1038/nchem.2632
ImpF: **23.0**

17. P. Dopieralski, J. Ribas–Arino, P. Anjukandi, M. Krupicka, D. Marx
Force-Induced Reversal of β-Eliminations: Stressed Disulfide Bonds in Alkaline Solution
Angew. Chem. Int. Ed. 55, 1304–1308 (**2016**) doi:10.1002/anie.201508005
ImpF: **11.3**

16. P. Anjukandi, P. Dopieralski, J. Ribas–Arino, D. Marx
The Effect of Tensile Stress on the Conformational Free Energy Landscape of Disulfide Bonds
PLOS One 9(10):e108812 (**2014**) DOI: 10.1371/journal.pone.0108812
ImpF: **3.5**

15. L. Walewski, P. Dopieralski, O. V. Shishkin, Z. Latajka
Quantum Delocalization of Benzene in the Ring Puckering Coordinates
Int. J. Quantum. Chem. 114, 534–542 (**2014**) DOI: 10.1002/qua.24606
ImpF: **1.4**

14. P. Dopieralski, J. Ribas–Arino, P. Anjukandi, M. Krupicka, J. Kiss, D. Marx
The Janus-faced role of external forces in mechanochemical disulfide bond cleavage
Nat. Chem. 5, 685–691 (**2013**) doi:10.1038/NCHEM.1676
ImpF: **20.5**

13. O.V. Shishkin, P. Dopieralski, I.V. Omelchenko, L. Gorb, Z. Latajka, J. Leszczynski
Entropy versus aromaticity in the conformational dynamics of aromatic rings
J. Mol. Model. (**2012**) doi:10.1007/s00894-012-1670-2
ImpF: **1.8**

12. O.V. Shishkin, P. Dopieralski, I.V. Omelchenko, L. Gorb, Z. Latajka, J. Leszczynski
Dynamical Non-Planarity of Benzene. Evidences from the Car–Parrinello Molecular Dynamics Study
J. Phys. Chem. Lett. 2, 2881 (**2011**) doi:10.1021/jz201327t
ImpF: **6.2**

11. P. Dopieralski, C.L. Perrin, Z. Latajka
On the intramolecular hydrogen bond in solution. Car-Parrinello and Path Integrals Molecular Dynamics perspective
J. Chem. Theory Comput. 7, 3505 (**2011**) doi:10.1021/ct200580c
ImpF: **5.1**

10. P. Dopieralski, J. Ribas–Arino, D. Marx
Force–transformed Free Energy Surfaces and Trajectory Shooting Simulations Reveal the Mechano–stereochemistry of Cyclopropane Ring–opening Reactions
Angew. Chem. Int. Ed. 50, 7105 (**2011**) doi:10.1002/anie.201100399
ImpF: **12.7**

9. P. Dopieralski, A. Burakowski, Z. Latajka, I. Olovsson
Hydration of $NaHCO_3$, $KHCO_3$, $(HCO_3^-)_2$, HCO_3^- and $CO_3{}^{2-}$ from Molecular Dynamics Simulation and Speed of Sound Measurements
Chem. Phys. Lett. 507, 89 (**2011**) doi:10.1016/j.cplett.2011.03.065
ImpF: **2.3**

8. P. Dopieralski, P. Anjukandi, M. Rueckert, M. Shiga, J. Ribas–Arino, D. Marx
On the role of polymer chains in transducing external mechanical forces to benzocyclobutene mechanophores
J. Mat. Chem. 21, 8309 (**2011**) doi:10.1039/C0JM03698F
ImpF: **5.1**

7. P. Dopieralski, Z. Latajka, I. Olovsson
Proton transfer dynamics in crystalline maleic acid from molecular dynamics calculations
J. Chem. Theory Comput. 6, 1455 (**2010**) doi:10.1021/ct100078w
ImpF: **5.1**

6. O.V. Shishkin, P. Dopieralski, G.V. Palamarchuk, Z. Latajka
Rotation around glycosidic bond as driving force of proton transfer in protonated 2–deoxyriboadenosine monophosphate (AMP)
Chem. Phys. Lett. 490, 221 (**2010**) doi:10.1016/j.cplett.2010.03.044
ImpF: **2.3**

5. P. Dopieralski, Z. Latajka, I. Olovsson
Proton transfer dynamics in the $(HCO_3^-)_2$ dimer of $KHCO_3$ from Car-Parrinello and Path Integrals molecular dynamics calculations
Acta Cryst. B66, 222 (**2010**) doi:10.1107/S0108768110002314
ImpF: **1.8**

4. P. Dopieralski, J. Panek, K. Mierzwicki, Z. Latajka, H. Ratajczak, A. Barnes
Theoretical study on the polarizability and hyperpolarizability of hydrogen bonded complexes of nitropyridines with hydrogen fluoride
J. Mol. Struct. THEOCHEM 916, 72 (**2009**) doi:10.1016/j.theochem.2009.09.008
ImpF: **1.3**

3. P. Dopieralski, Z. Latajka, I. Olovsson,
Proton distribution in $KHCO_3$ from ab initio Molecular Dynamics simulation
Chem. Phys. Lett. 476, 223 (**2009**) doi:10.1016/j.cplett.2009.06.048
ImpF: **2.3**

2. P. Dopieralski, J. Panek, Z. Latajka,
First-principles investigation on isomerization by proton transfer in beta-fumaric acid crystal
J. Chem. Phys. 130, 164517 (**2009**) doi:10.1063/1.3124192
ImpF: **2.9**

1. H. Ratajczak, A.J. Barnes, J. Baran, A.M. Yaremko, Z. Latajka, P. Dopieralski,
Anharmonic interactions and infrared bandshape of the hydrogen bond vibration of potassium hydrogen (deuterium) maleate crystals
J. Mol. Struct. 887, 9 (**2008**) doi:10.1016/j.molstruc.2007.10.005
ImpF: **1.6**

Grants and Awards

2017–2018	National Science Center, Poland (NCN) GRANT No. 2016/23/B/ST4/01099 240 800PLN *Studies on temperature dependance of effective H and D atom sizes in crystal phase by ab initio molecular dynamics*
2016–2017	Jülich JUQUEEN Computer Grant *Mechanochemistry of covalent bond breaking from first principles simulations* (Renewal)
2015–2017	National Science Center, Poland (NCN) GRANT No. 2014/13/B/ST4/05009 443 340PLN *Understanding disulfides reactivity - mechanochemical perspective*
2014–2017	National Science Center, Poland (NCN) Award for Young Outstanding Scientist
2014	The Award of the Rector of the University of Wroclaw for scientific achievements in 2013
2015–2015	Internal Grant for Young Scientists, Ministry of Science and Higher Education of Poland (MNiSzW) *Is Deuter always smaller than Hydronium? Theoretical investigations by ab initio Molecular Dynamics*
2012–2015	Jülich JUQUEEN Computer Grant *Mechanochemistry of covalent bond breaking from first principles simulations* (Renewal)
2011	Team Award of the Rector of the University of Wroclaw for scientific achievements in 2010
2011–2012	Jülich JUGENE Computer Grant *Mechanochemistry of covalent bond breaking from first principles simulations* (Renewal)

2011–2012	Internal Grant for Young Scientists, Ministry of Science and Higher Education of Poland (MNiSzW) GRANT No. 105/10/E-344/M/2011 *Counterions influence on the solvation of simple organic ions - Molecular Dynamics study*
2010–2011	Jülich JUGENE Computer Grant *Mechanochemistry of covalent bond breaking from first principles simulations*
2008–2010	Ministry of Science and Higher Education of Poland (MNiSzW) GRANT No. NN2040958833 *Proton dynamics of hydrogen bonded model systems– theoretical study*
2007	Grant of Deutsche-Polnische Gesellschaft der Universität Wroclaw
2006	HPC-EUROPA GRANT: HPC04KJFHW RII3-CT-2003-506079 Ruhr-University Bochum, Prof. Dominik Marx

Conferences, Workshops

09.2017 HBOND2017 - Horizons in Hydrogen Bond Research, Jyvaskyla, Finland, Invited Speaker
Stressed Disulfides Bonds in Alkaline Solution

08.2017 11^{nd} Triennial Congress of the World Association of Theoretical and Computational Chemistry, Munich, Germany, Speaker
Stressed Disulfides Bonds in Alkaline Solution

09.2016 52^{nd} Symposium on Theoretical Chemistry, Bochum, Germany,
Stressed Disulfides Bonds in Alkaline Solution

09.2013 International Symposium on Mechanochemistry in Synthesis and Nanoscience, Lochow, Poland,
Force as Dr. Jekyll and Mr. Hyde

09.2013 CPMD Meeting 2013, Leipzig, Germany,
Molecular Dynamics Perspective On the Intramolecular Hydrogen Bond in Solution

08.2013 ISTCP-VIII, The Congress of the International Society of Theoretical Chemical Physics, Budapest, Hungary,
Mechanochemistry: The curious case of cyclopropane

06.2013 International Opening Symposium of the Cluster of Excellence RESOLV, Bochum, Germany,

07.2012 Workshop: Introduction into the Blue Gene/Q architecture, Jülich, Germany

02.2012 6^{th} NIC Symposium, Jülich, Germany

09.2011 CPMD2011: Extending the limits of Ab initio Molecular Dynamics Simulations for Chemistry, Materials Science and Biophysics, Barcelona, Spain
Force-Transformed Free Energy Surfaces

01.2011 15^{th} International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Trieste, Italy
Mechanochemistry

07.2010 Modeling and Design of Molecular Materials 2010, Wroclaw, Poland
Mechanochemistry. The road to understanding

06.2008	Conference on Modeling and Computation of Structure and Dynamics of Condensed Phase Systems, Trieste, Italy *New possible mechanism to obtain fumaric acid isomers*
09.2007	Horizons in Hydrogen Bond, St. Petersburg, Russia *Quantum Dynamics Investigation on Proton Transfer in dicarboxilic acid crystals*
04.2006	III International Conference on Hydrogen Bonding and Molecular Interactions, Kyiv, Ukraine *Car-Parrinello Molecular Dynamics and Path Integrals Molecular Dynamics of Dicarboxilic Acid Crystals*
06.2004	School of Organic Physical Chemistry in Polanica Zdroj, Poland *Theoretical study on the polarizability and hyperpolarizability of hydrogen bonded complexes*