List of Publications of
Dr. Pavlo O. Dral

Peer-Reviewed Articles

18. Bettina D. Gliemann, Ana G. Petrovic, Eva M. Zolnhofer, **Pavlo O. Dral**, Frank Hampel, Georg Breitenbruch, Schulze Philipp, Vijay Raghavan, Karsten Meyer, Prasad L. Polavarapu, Nina Berova, Milan Kivala, Configurationally Stable Chiral Dithia-Bridged Hetero[4]helicene Radical Cation: Electronic Structure and Absolute Configuration. *Chem. Asian J.* **2017**, *12*, 31–35. DOI: 10.1002/asia.201601452.
17. Jakob F. Hitzenberger, **Pavlo O. Dral**, Ute Meinhardt, Timothy Clark, Walter Thiel, Milan Kivala, Thomas Drewello, Stability of Odd- Versus Even-Electron Gas-Phase (Quasi)Molecular Ions Derived from Pyridine-Substituted N-Heterotriangulenes. *ChemPlusChem* **2017**, *82*, 204–211. DOI: 10.1002/cplu.201600416.
    Appeared as the front cover in ChemPlusChem (p. 161, DOI: 10.1002/cplu.201600597) with the associated cover profile (p. 163, DOI: 10.1002/cplu.201600596).
16. Gerhard König, Frank C. Pickard IV, Jing Huang, Andrew C. Simmonett, Florentina Tofoleanu, Juyong Lee, **Pavlo O. Dral**, Samarjeet Prasad, Michael Jones, Yihan Shao, Walter Thiel, Bernard R. Brooks, Calculating Distribution Coefficients Based on Multi-Scale Free Energy Simulations: An Evaluation of MM and QM/MM Explicit Solvent Simulations of Water-Cyclohexane Transfer in the SAMPL5 Challenge. *J. Comput. Aided Mol. Des.* **2016**, *30*, 989–1006. DOI: 10.1007/s10822-016-9936-x.
15. Ute Meinhardt, Fabian Lodermeyer, Tobias A. Schaub, Andreas Kunzmann, **Pavlo O. Dral**, Anna Chiara Sale, Frank Hampel, Dirk M. Guldi, Ruben D. Costa, Milan Kivala, *N*-Heterotriangulene Chromophores with 4-Pyridyl Anchors for Dye-Sensitized Solar Cells. *RSC Adv.* **2016**, *6*, 67372–67377. DOI: 10.1039/C6RA14799B.
14. **Pavlo O. Dral**, Xin Wu, Lasse Spörkel, Axel Koslowski, Walter Thiel, Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks for Ground-State Properties. *J. Chem. Theory Comput.* **2016**, *12*, 1097–1120. DOI: 10.1021/acs.jctc.5b01047.
13. **Pavlo O. Dral**, Xin Wu, Lasse Spörkel, Axel Koslowski, Wolfgang Weber, Rainer Steiger, Mirjam Scholten, Walter Thiel, Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Theory, Implementation, and Parameters. *J. Chem. Theory Comput.* **2016**, *12*, 1082–1096. DOI: 10.1021/acs.jctc.5b01046.

12. Raghunathan Ramakrishnan, **Pavlo O. Dral**, Matthias Rupp, O. Anatole von Lilienfeld, Big Data Meets Quantum Chemistry Approximations: The Δ-Machine Learning Approach. *J. Chem. Theory Comput.* **2015**, *11*, 2087–2096. DOI: 10.1021/acs.jctc.5b00099.
arXiv:1503.04987 [physics.chem-ph].
11. **Pavlo O. Dral**, O. Anatole von Lilienfeld, Walter Thiel, Machine Learning of Parameters for Accurate Semiempirical Quantum Chemical Calculations. *J. Chem. Theory Comput.* **2015**, *11*, 2120–2125. DOI: 10.1021/acs.jctc.5b00141.
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7. Hui Li, Christina Schubert, **Pavlo O. Dral**, Rubén Costa, Andrea La Rosa, Jürg Thüring, Shi-Xia Liu, Chenyi Yi, Salvatorre Filippone, Nazario Martin, Silvio Decurtins, Timothy Clark, Dirk M. Guldi, Probing Charge Transfer in Benzodifuran–C_{60} Dumbbell-Type Electron Donor–Acceptor Conjugates: Ground- and Excited-State Assays. *ChemPhysChem* **2013**, *14*, 2910–2919. DOI: 10.1002/cphc.201300378.
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4. **Pavlo O. Dral**, Theoretical study of electronic properties of carbon allotropes. *Friedrich-Alexander-Universität Erlangen-Nürnberg*, Dissertation (Dr. rer. nat.), **2013**, http://opus4.kobv.de/opus4-fau/frontdoor/index/index/docId/3763.
3. **Pavlo O. Dral**, Comparative DFT and Ab Initio Study of Nitrogen-Containing Electrophiles. *Department of Organic Chemistry and Organic Compounds, National Technical University of Ukraine "Kiev Polytechnic Institute"*, Magister dissertation, **2010**.
2. **Pavlo O. Dral**, Hydrogen Chemisorption on Neutral and Electron-Doped Graphenic Surfaces: A Theoretical Investigation. *Friedrich-Alexander-Universität Erlangen-Nürnberg*, Master thesis, **2010**.
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Talks

10 **Pavlo O. Dral**, *Machine Learning for Predicting Accurate Quantum Chemical Energies*. 2016 AIChE Annual Meeting, San Francisco, USA, November 13–18, 2016.

9 **Invited talk: Pavlo O. Dral**, *Fast Simulations of Excited States at Different Scales*. Excited States Simulations: Bridging Scales workshop, Marseille, France, November 7–10, 2016.

8 **Pavlo O. Dral**, Walter Thiel, *The Quest for Accurate Semiempirical Methods*. The 29th Molecular Modeling Workshop 2015, Erlangen, Germany, March 9–11, **2015**; p. 33.

7 **Pavlo O. Dral**, Timothy Clark, *UNO–CAS Calculations of Band Gaps of Carbon Systems*. Klausurtagung des SFB 953, Bad Staffelstein, Germany, April 27–29, **2012**.

6 **Pavlo O. Dral**, Timothy Clark, *Application of Semiempirical UNO–CI and CI Methods in Nanoelectronics*. The 26th Molecular Modelling Workshop, Erlangen, Germany, March 12–14, **2012**; p. 39.

5 **Pavlo O. Dral**, Timothy Clark, *Modeling Molecular Electronic Properties with Semiempirical UNO–CAS*. The 25th Molecular Modelling Workshop, Erlangen, Germany, April 4–6, **2011**; p. 25.

4 **Pavlo O. Dral**, Tatyana E. Shubina, Andreas Hirsch, Timothy Clark, *Hydrogenation of Fullerene C_{60}: A Theoretical Investigation*. The 13th JungChemikerForum Spring Symposium, Erlangen, Germany, March 23–26, **2011**; p. 36.

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2 **Pavlo O. Dral**, Andrey A. Fokin, *Quantum-Mechanical Computations of Alkane Nitrolysis*. The 1st International (3rd All-Ukrainian) Theoretical and Practical Conference of Students, Postgraduates and Young Scientists in Chemistry and Chemical Technology, Kiev, Ukraine, April 23–25, **2008**.

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20 **Pavlo O. Dral**, Alec Owens, Walter Thiel, *Machine Learning for Calculating Accurate Potential Energy Surfaces*. 52nd Symposium on Theoretical Chemistry 2016 "Chemistry in Solution", Bochum, Germany, September 26–29, **2016**; P52.

19 **Pavlo O. Dral**, Walter Thiel, *Improving the Accuracy of Fast Methods*. The 8th Molecular Quantum Mechanics, Uppsala, Sweden, June 26 – July 1, **2016**; p. 151.

18 **Pavlo O. Dral**, Walter Thiel, *Improved Semiempirical Methods*. The 51th Symposium on Theoretical Chemistry 2015 "Chemistry in Motion", Potsdam, Germany, September 20–24, **2015**; P 201.

17 **Pavlo O. Dral**, Raghunathan Ramakrishnan, Matthias Rupp, Walter Thiel, O. Anatole von Lilienfeld, *Combining Semiempirical Quantum Mechanics with Machine Learning: Towards Hybrid Quantum Mechanics/Machine Learning (QM/ML).* The 50th Symposium on Theoretical Chemistry 2014 "Quantum Chemistry and Chemical Dynamics", Vienna, Austria, September 14–18, **2014**; P225.

16 **Pavlo O. Dral**, *The Unrestricted Local Properties as a Useful Tool for Nanoelectronics*. Workshop QuantumHagen on Modeling of Electronic Devices and Materials at the Nanoscale, Copenhagen, Denmark, July 1–3, **2014**; p. 31.

15 **Pavlo O. Dral**, Christina Schubert, Milan Kivala, Dirk M. Guldi, Timothy Clark, *Photoinduced Electron Transfer in Donor–Acceptor Nanosystems: A Theoretical Study*. The 2nd Erlangen Symposium on Synthetic Carbon Allotropes, Erlangen, Germany, September 29 – October 2, **2013**; p. 78.

14 Volker Strauß, Bettina Gliemann, Jakob Hitzenberger, **Pavlo O. Dral**, Jean-Paul Gisselbrecht, Thomas Drewello, Timothy Clark, Dirk M. Guldi, Milan Kivala, *Cooperative Fluorescence – Triphenylamine-Tetrathiafulvalene Hybrids as Electron-Rich Receptors for Fullerenes*. The 2nd Erlangen Symposium on Synthetic Carbon Allotropes, Erlangen, Germany, September 29 – October 2, **2013**; p. 56.

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12 **Pavlo O. Dral**, Tatyana E. Shubina, Laura Gagliardi, Dirk M. Guldi, Timothy Clark, *A Possible Synthesis and the Unusual Electronic Properties of Endofullerene* $NH_4^+@C_{60}$

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11 Maximilian Kriebel, **Pavlo O. Dral**, Johannes Margraf, Christof Jäger, Thilo Bauer, Timothy Clark, *Time-Dependent Propagation on Electron Affinity Landscapes.* The 49th Symposium on Theoretical Chemistry "Bridging Scales in Theoretical Chemistry", Erlangen, Germany, September 22 – 26, **2013**, P-114.

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6 **Pavlo O. Dral**, Timothy Clark, *UNO–CI calculations of electronic transitions in nanosystems*. Modeling and Design of Molecular Materials 2012, Wrocław, Poland, September 10–14, **2012**; P11A.

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4 Dmytro I. Sharapa, **Pavlo O. Dral**, Tatyana E. Shubina, Timothy Clark, *Charge transfer in Fe-intercalated SWCNT*. The 26th Molecular Modelling Workshop, Erlangen, Germany, March 12–14, **2012**; p. 79.

3 Igor. A. Levandovskiy, **Pavlo O. Dral**, Tatyana E. Shubina, Boris V. Chernyaev, *QSRR Studies of Methylnaphtalines Adsorption on Silver-Ion Stationary Phase*. Methods and Applications of Computational Chemistry. Third International Simposium, Odessa, Ukraine, June 28 – July 2, **2009**; p. 83.

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Programs

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