Dr. Jan Wenzel

Scientist Computational and Systems Toxicology

Sanofi-Aventis Deutschland GmbH
R&D, Preclinical Safety – Global Operations Germany

Jan Wenzel studied chemistry at the Goethe University Frankfurt, focusing research projects in computational quantum chemistry. His PhD was received from the University of Heidelberg, where he conducted fundamental research for simulation of X-ray absorption spectroscopy. Afterwards, Jan started as PostDoc at Sanofi in Frankfurt. The project's focus was on deep learning in the field of safety big data analytics, to advance the capabilities to analyze, predict and optimize safety parameters of novel drug candidates. Currently, Jan is Scientist for computational and systems toxicology at Sanofi.

List of Publications

1. Wenzel, J.; Matter, H.; Schmidt, F., Predictive Multitask Deep Neural Network Models for ADME-Tox Properties: Learning from Large Datasets, *submitted for publication* **2018**
2. Wenzel, J.; Anger, L.; Amberg, A.; Matter, H.; Hessler, G.; Griesang, N.; Mertsch, K.; Czich, A.; Schmidt, F., Enhancing compound safety assessment using "Multitask" deep neural nets. *Toxicol. Lett.* **2018**, 295.
3. Miteva, T.; Kryzhevoi, N. V.; Sisourat, N.; Nicolas, C.; Pokapanich, W.; Saisopa, T.; Songsiriritthigul, P.; Rattanachai, Y.; Dreuw, A.; Wenzel, J.; et al., The All-Seeing Eye of Resonant Auger Electron Spectroscopy: A Study on Aqueous Solution Using Tender X-rays. *J. Phys. Chem. Lett.* **2018**, 9, 4457-4462.
4. Wenzel, J.; Dreuw, A., Physical Properties, Exciton Analysis, and Visualization of Core-Excited States: An Intermediate State Representation Approach. *J. Chem. Theory Comput.* **2016**, 12, 1314-30.
5. Wenzel, J. Development and Implementation of Theoretical Methods for the Description of Electronically Core-Excited States. Dissertation, Heidelberg University, Heidelberg, 2016.
6. Schmidt, N.; Wenzel, J.; Dreuw, A.; Fink, R. H.; Hieringer, W., Matrix effects in the C 1s photoabsorption spectra of condensed naphthalene. *J. Chem. Phys.* **2016**, 145, 234307.
7. Miteva, T.; Wenzel, J.; Klaiman, S.; Dreuw, A.; Gokhberg, K., X-Ray absorption spectra of microsolvated metal cations. *PCCP* **2016**, 18, 16671-81.
8. Wenzel, J.; Holzer, A.; Wormit, M.; Dreuw, A., Analysis and comparison of CVS-ADC approaches up to third order for the calculation of core-excited states. *J. Chem. Phys.* **2015**, 142, 214104.
9. Shao, Y.; Gan, Z.; Epifanovsky, E.; Gilbert, A. T. B.; Wormit, M.; et al., Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Mol. Phys.* **2015**, 113, 184-215.
10. Plasser, F.; Thomitzni, B.; Bappler, S. A.; Wenzel, J.; Rehn, D. R.; Wormit, M.; Dreuw, A., Statistical analysis of electronic excitation processes: Spatial location, compactness, charge transfer, and electron-hole correlation. *J. Comput. Chem.* **2015**, 36, 1609-20.
11. Wormit, M.; Rehn, D. R.; Harbach, P. H. P.; Wenzel, J.; Krauter, C. M.; Epifanovsky, E.; Dreuw, A., Investigating excited electronic states using the algebraic diagrammatic construction (ADC) approach of the polarisation propagator. *Mol. Phys.* **2014**, 112, 774-784.
12. Wenzel, J.; Wormit, M.; Dreuw, A., Calculating core-level excitations and X-ray absorption spectra of medium-sized closed-shell molecules with the algebraic-diagrammatic construction scheme for the polarization propagator. *J. Comput. Chem.* **2014**, 35, 1900-15.
13. Wenzel, J.; Wormit, M.; Dreuw, A., Calculating X-ray Absorption Spectra of Open-Shell Molecules with the Unrestricted Algebraic-Diagrammatic Construction Scheme for the Polarization Propagator. *J. Chem. Theory Comput.* **2014**, 10, 4583-98.
14. Wenzel, J.; Dreuw, A.; Burghardt, I., Charge and energy transfer in a bithiophene perylenediimide based donor-acceptor-donor system for use in organic photovoltaics. *PCCP* **2013**, 15, 11704-16.