Physical and Computational Chemistry
Spring 2025 (C. Corminboeuf)

Presentation of an article linked to computational organic chemistry

A. Paper of your choice (to be approved first)

or

B. Article from the following list

Theoretical Chemistry

- M. G. Medvedev, I. S. Bushmarinov, J. Sun, J. P. Perdew, and K. A. Lyssenko, *Density functional theory is straying from the path toward the exact functional, Science* **2017**, *355*, 49.
- **Only for the concept of atomic charges**: J. F. Gonthier, S. N. Steinmann, M. D. Wodrich, and C. Corminboeuf, Quantification of *"Fuzzy" Chemical Concepts: A Computational Perspective*, *Chem. Soc. Rev*. **2012**, *41*, 4671.
- Y. Minenkov, G. Occhipinti, and V. R. Jensen, *Metal-Phosphine Bond Strengths of the Transition Metals: A Challenge for DFT*, *J. Phys. Chem. A* **2009**, *113*, 11833.
- N. Rahat, E. Kraisler, *Plateaus in the Potentials of Density-Functional Theory: Analytical Derivation and Useful Approximations.*, *J. Chem. Theory Comput.* **2025**. ASAP.

Reaction/Rearrangement Mechanisms

- A. Seegerer, J. Hioe, M. M. Hammer, F. Morana, P. J. W. Fuchs, and R. M. Gschwind, Remote-Stereocontrol in Dienamine Catalysis: Z-Dienamine Preferences and Electrophile–Catalyst Interaction Revealed by NMR and Computational Studies, *J. Am. Chem. Soc*. **2016**, *138*, 9864–9873.
- R. E. Plata and D. A. Singleton, A Case Study of the Mechanism of Alcohol-Mediated Morita Baylis−Hillman Reactions. The Importance of Experimental Observations, *J. Am. Chem. Soc.* **2015**, *137*, 3811–3826.
- V. A. Roytman, S. Jin, V. T. Nguyen, V. D. Nguyen, G. C. Haug, O. V. Larionov, D. A. Singleton, *Bond Memory in Dynamically Determined Stereoselectivity. J. Am. Chem. Soc*. **2020**, *142*, 85.
- M. Zhu, C. Zheng, *Post-Spin Crossing Dynamics Determine the Regioselectivity in Open-Shell Singlet Biradical Recombination., Org. Chem. Front.* **2022**, *9*, 995.
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Physical Organic Chemistry

- D. S. Allgaüer, H. Jangra, H. Asahara, Z. Li, Q. Chen, H. Zipse, A. R. Ofial, and H. Mayr, Quantification and Theoretical Analysis of the Electrophilicities of Michael Acceptors, *J. Am. Chem. Soc.* **2017**, *139*, 13318−13329.

- S. E. Wheeler, *Local Nature of Substituent Effects in Stacking Interactions*, *J. Am. Chem. Soc*. **2011**, *133*, 10262–10274.
- S. Ehrlich, H. F. Bettinger, and S. Grimme, *Dispersion-Driven Conformational Isomerism in σ-Bonded Dimers of Larger Acenes*, *Angew. Chem. Int. Ed*. **2013**, *52*, 10892–10895.
- R. Pollice, P. Chen, *A Universal Quantitative Descriptor of the Dispersion Interaction Potential*., *Angew. Chem*. **2019**, *58*, 9758.
- J. P. Joyce, M. P. Shores, A. K. Rappè, *Protobranching as Repulsion-Induced Attraction: A Prototype for Geminal Stabilization., Phys. Chem. Chem. Phys*. **2020**, *22*, 16998.
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Catalysis

- S. Das, R. C. Turnell-Ritson, P. Dyson, C. Corminboeuf, *Design of Frustrated Lewis Pair Catalysts for Direct Hydrogenation of CO2*., *Angew. Chem. Int. Ed.* **2022**, *61*, e202208987.
- D. Yepes, F. Neese, B. List, and G. Bistoni, Unveiling the Delicate Balance of Steric and Dispersion Interactions in Organocatalysis Using High-Level Computational Methods, *J. Am. Chem. Soc*. **2020**, *142*, 3613–3625.
- J. G. Harrison, O. Gutierrez, N. Jana, T. G. Driver, and D. J. Tantillo, Mechanism of Rh_2(II)-Catalyzed Indole Formation: The Catalyst Does Not Control Product Selectivity, *J. Am. Chem. Soc*. **2016**, *138*, 487–490.
- Maji, Mallojjala, Wheeler, *Electrostatic Interactions in Asymmetric Organocatalysis. Acc Chem Res*. **2023,** *56*, 1990.

Machine Learning in Chemistry

- Guan, Coley, Wu, Ranasinghe, Heid, Struble, Pattanaik, Green, Jensen, "*Regio-Selectivity Prediction with a Machine-Learned Reaction Representation and on-the-Fly Quantum Mechanical Descriptors.", Chem. Sci.* **2021**, *12*, 2198.
- J. P. Janet and H. J. Kulik, *Predicting Electronic Structure Properties of Transition Metal Complexes with Neural Networks*, *Chem. Sci*. **2017**, *8*, 5137–5152.
- J. A. Hueffel, T. Sperger, I. Funes-Ardoiz, J. S. Ward, K. Rissanen, and F. Schoenebeck, *Accelerated Dinuclear Palladium Catalyst Identification Through Unsupervised Machine Learning*, Science **2021**, *374*, 1134–1140.
- G. Pesciullesi, P. Schwaller, T. Laino, and J. Reymond, *Transfer Learning Enables the Molecular Transformer to Predict Regio- and Stereoselective Reactions on Carbohydrates*, *Nat. Commun*. **2020**, *11*, 4874.
- Samha, Kara, Vogt, Odogwu, Elward, Crawford, Steves, Sigman, *Predicting success in Cu-catalyzed C–N coupling reactions using data science*., *Sci. Adv.* **2024** *10*, eadn3478.
- P. C. St. John, Y. Guan, Y. Kim, S. Kim, and R. S. Paton, *Prediction of Organic Homolytic Bond Dissociation Enthalpies at Near Chemical Accuracy with Sub-Second Computational Cost*, *Nat. Commun*. **2020**, *11*, 2328.

- Schleinitz, Carretero-Cerdán, Gurajapu, Harnik, Lee, Pandey, Milo, Reisman, *Designing Target-Specific Data Sets for Regioselectivity Predictions on Complex Substrates. J. Am. Chem. Soc.* **2025**, *147*, 7476.
- S. Gallarati, P. van Gerwen, R. Laplaza, L. Brey, A. Makaveev, C. Corminboeuf, "*A Genetic Optimization Strategy with Generality in Asymmetric Organocatalysis as a Primary Target. Chem. Sci.* **2024**, *15*, 3640.