chemisch
physikalische
gesellschaft

Gegründet im Jahre 1869 von H. Hlasiwetz, J. Loschmidt, J. Petzval und J. Stefan

EINLADUNG

zum Vortrag von

Prof. Dr. Esther Heid

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Tailoring Machine Learning to Chemistry

am Dienstag, 27. Mai 2025, um 17:30 Uhr

Ort: Lise-Meitner-Hörsaal, Fakultät für Physik, Universität Wien,
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

Barrierefreier Zugang: Boltzmanngasse 5, Lift, 1. Stock rechts über den Gang zum Hintereingang des Hörsaals

Abstract:

Machine learning has become a powerful tool for predicting and even designing molecular properties, materials, and chemical reactions. By nature, machine learning is data-driven; it aims to uncover complex patterns, such as the solubility or antibiotic activity of a compound, directly from its structure. However, generating large, high-quality chemical datasets is often expensive and time-consuming, making the development of data-efficient models a key focus in the field. Successful predictions typically rely on machine learning architectures that incorporate domain knowledge, such as the chemical and physical symmetries of a system. But how much can such models actually support the day-to-day work of a chemist?

In this talk, I will provide an overview of the field and present my work on modeling molecular properties,[1] reaction properties,[2] retrosynthesis,[3] and enzymatic reactions,[4,5] together with an evaluation of their practical impact and usability. I will also discuss the challenge of quantifying uncertainty in chemical machine learning,[6,7] that is, evaluating the reliability of predictions of a model. Finally, I will discuss my current research efforts aimed at advancing more sustainable chemistry through machine learning, with a focus on predicting chemical reactions with and without catalysts.

[1] E. Heid, K. P. Greenman, Y. Chung, S.-C. Li, D. E. Graff, F. H. Vermeire, H. Wu, W. H. Green, and C. J. McGill. *J. Chem. Inf. Model.*, **2023**, *64*, 9–17.

[2] E. Heid and W. H. Green. *J. Chem. Inf. Model.*, **2021**, *62*, 2101–2110.

[3] E. Heid, J. Liu, A. Aude and W. H. Green. *J. Chem. Inf. Model.*, **2021**, *62*, 16–26.

[4] E. Heid, D. Probst, W. H. Green and G. K. H. Madsen. *Chem. Sci.*, **2023**, *14*, 14229– 14242.

[5] E. Heid, S. Goldman, K. Sankaranarayanan, C. W. Coley, C. Flamm and W. H. Green. *J. Chem. Inf. Model.*, **2021**, *61*, 4949–4961.

[6] E. Heid, J. Schorghuber, R. Wanzenbock and G. K. H. Madsen. *J. Chem. Inf. Model.*, **2024**, *64*, 6377–6387.

[7] E. Heid, C. J. McGill, F. H. Vermeire and W. H. Green. *J. Chem. Inf. Model.*, **2023**, *63*, 4012–4029.

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