Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

**Institute for Molecular Physical Science (IMPS)**

# Einladung zu einem Kolloquium

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| Datum/Zeit: | **Dienstag, 01.04.2025, 16.45 Uhr** |
| Referent: | **Prof. Konstantinos Vogiatzis**<br>University of Tennessee, Knoxville, USA |
| Titel: | *Exploration of the Electron Correlation Space with Data-driven Quantum Chemistry* |
| Ort: | **HCI G7** |

Our research focuses on developing data-driven computational methodologies that bridge the gap between quantum chemistry and machine learning (ML) to overcome the size limitations inherent in highly accurate yet computationally intensive methods such as coupled-cluster (CC) theory. Specifically, we have advanced a data-driven coupled-cluster singles and doubles (DDCCSD) model, which demonstrates significant speedup and transferability compared to conventional approaches. [1-3] However, a key challenge for DDCC models lies in the exponential growth of training set sizes with increasing system complexity. To address this, we explored five amplitude selection techniques that effectively sample the amplitude space, reducing the data requirements for training while mitigating model overfitting. [4] These strategies enhance the applicability of DDCCSD to larger molecular systems and more extensive basis sets. We will also discuss extensions of this methodology, including perturbative triples (T) corrections [5] and the incorporation of graph neural network architectures. Notably, our recent development of a physics-informed neural network for DDCC achieved a ten-fold increase in accuracy compared to earlier models, marking a substantial improvement in predictive capabilities. We will also outline the current limitations of these methods and propose potential solutions to address them. Additionally, we have extended our framework to other quantum chemical methods designed to handle strong electron correlation, such as the variational 2-electron reduced density matrix complete active space self-consistent field (v2RDM-CASSCF) method. [6]

[1] J. Townsend, K. D. Vogiatzis, *J. Phys. Chem. Lett.*, **2019**, *10*, 4129.
[2] J. Townsend, K. D. Vogiatzis, *J. Chem. Theory Comput.*, **2020**, *16*, 7453.
[3] G. M. Jones, P. D. V. S. Pathirage, K. D. Vogiatzis, Data-driven Acceleration of Coupled-Cluster Theory and Perturbation Theory Methods, in: “Quantum Chemistry in the Age of Machine Learning”, **2022**, Editor: Pavlo Dral, Elsevier, pp. 509-529.
[4] P. D. V. S. Pathirage, J. T. Phillips, K. D. Vogiatzis, *J. Phys. Chem. A*, **2024**, *128*, 1938.
[5] P. D. V. S. Pathirage, S. Akram, B. Quebedeaux, K. D. Vogiatzis, *In Revision*.
[6] G. M. Jones, R. R. Li, A. E. DePrince III, K. D. Vogiatzis, *J. Phys. Chem. Lett.*, **2023**, *14*, 6377.

**Gäste sind willkommen**