# Workshop "Machine Learning for Chemistry and Chemical Engineering (ML4CCE)", September 9th, 2024

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| 09:00 | **Opening Remarks** |
| 09:15 | **Keynote Talk by Felix Strieth-Kalthoff**: *Machine Learning Hits the Lab: Experiment Planning with Bayesian (Co-)Pilots* |
| 10:00 | **Johannes Zenn**: *Balancing Molecular Information and Empirical Data in the Prediction of Physico-Chemical Properties* |
| 10:15 | **Nicolas Hayer**: *Embedding Machine Learning Methods in Physical Thermodynamic Models* |
| 10:30 | **Mayank Nagda**: *PITs: Physics-Informed Transformers for Predicting Chemical Phenomena* |
| 10:45 | **Stephen O. Obonyo**: *Decoding Molecular Language Model with Beam Search* |
| 11:00 | **Coffee Break** |
| 11:30 | **Keynote Talk by Dominik Grimm**: *Automated Flowsheet Synthesis with Deep Reinforcement Learning* |
| 12:15 | **Poster Session I**: all posters with **odd** numbers |
| 13:00 | **Lunch Break** |
| 14:00 | **Keynote Talk by Venkat Venkatasubramanian**: *Do Large Language Models "Understand" Their Knowledge?* |
| 14:45 | **Best Paper Talk by Gabriel Cathoud**: *Insights into Chemistry: Explainable AI with Group Contribution in Graph Neural Networks* |
| 15:10 | **Poster Session II**: all posters with **even** numbers |
| 16:00 | **Coffee Break** |
| 16:30 | **Sagar Srinivas Sakhinana**: *Towards Human-Level Understanding of Complex Process Engineering Schematics: A Pedagogical Introspective Multi-Agent Framework for Open-Domain Question Answering* |
| 16:45 | **Eduardo F. Montesuma**: *Benchmarking Domain Adaptation for Chemical Processes on the Tennessee Eastman Process* |
| 17:00 | **Closing Remarks** |

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## Poster Session I
12:15-13:00

1 **Diogo R. Ferreira**
*Machine Learning for Chemistry Reduction in $N_2$-$H_2$ Low-Temperature Plasmas*

3 **Marco Hoffmann**
*Graph Neural Networks with Molecular Interaction Pooling for Pure-Component Vapor Pressure Prediction*

5 **Johannes Zenn**
*Balancing Molecular Information and Empirical Data in the Prediction of Physico-Chemical Properties*

7 **Nicolas Hayer**
*Embedding Machine Learning Methods in Physical Thermodynamic Models*

9 **Arjun John Kaithakkal**
*Understanding CNN-Based Shape Optimization for Thermo-Hydraulic Efficiency Using Explainable Deep Learning*

11 **Daniel Reinhardt**
*cPAX: Comparative Visualization of Known and Novel Anomalies for Monitoring Chemical Plants*

13 **Jens Wagner**
*Deep Set Models for Elucidating Unknown Mixtures with NMR Spectroscopy*

15 **Mayank Nagda**
*PITs: Physics-Informed Transformers for Predicting Chemical Phenomena*

17 **Justus C. Will**
*Enhancing Realism in Batch Distillation Simulations: Data-Efficient Time Series Style Transfer with Transformers*

19 **Marius J. Peter**
*Anomaly Classification of Tennesee Eastman Process Data*

21 **Luisa Peterson**
*Surrogate Modeling of Dynamical Systems: Deep Learning or Model-Order Reduction?*

23 **Sagar Srinivas Sakhinana**
*Towards Human-Level Understanding of Complex Process Engineering Schematics: A Pedagogical, Introspective Multi-Agent Framework for Open-Domain Question Answering*

## Poster Session II
15:10-16:00

2 **Ali Can Kara**
*ChemGraph Explainer: A Graphical User Interface for Explaining Predictions of Graph Neural Networks in Chemistry*

4 **Gabriel Cathoud**
*Insight into Chemistry: Explainable AI with Group Contribution in Graph Neural Networks*

6 **Jan G. Rittig**
*Structuring Latent Spaces of Variational Autoencoders for Molecular Design*

8 **Manuel Borja**
*Modelling Tablet Quality Attributes Using Probabilistic, Knowledge-Guided Neural Network*

10 **Zeno Romero**
*Prediction of Diffusion Coefficients in Mixtures with Tensor Completion*

12 **Viktor Martinek**
*Shape Constraints in Symbolic Regression Using Penalized Least Squares*

14 **Dean Brandner**
*Optimizing Operation Recipes with Reinforcement Learning for Safe and Interpretable Control of Chemical Processes*

16 **Eduardo F. Montesuma**
*Benchmarking Domain Adaptation for Chemical Processes on the Tennessee Eastman Process*

18 **Justus Arweiler**
*Anomaly Detection on Experimental Chemical Process Data*

20 **Fabian Hartung**
*Deep Anomaly Detection on Tennesse Eastman Process Data*

22 **Simon Lutz**
*A Benchmark Suite for Neural Network Verification*

24 **Sagar Srinivas Sakhinana**
*Retrieval-Augmented Instruction Tuning for Automated Process Engineering Calculations: A Tool-Chaining Problem-Solving Framework with Attributable Reflection*