SCS Symposium on AI 2024
«Critical Use of AI in Chemistry»

On November 25th, 2024, the first symposium in a series of events on 'Critical use of AI in Chemistry' will take place at University of Fribourg. The focus of this first event is on the use of AI in Quantum Chemistry.

The rapid progress of Artificial Intelligence (AI) is transforming nearly every facet of our society and scientific research, with Quantum Chemistry not being an exception. AI transforms this field, rapidly impacting molecular and material simulations at various scales. A critical examination of AI applications in Quantum Chemistry is essential to discern areas where AI can significantly contribute and identify realms where current AI approaches fall short. The conference will explore AI's dual role in advancing Quantum Chemistry by enhancing developments and accelerating quantum chemistry through AI surrogate models replicating its methods.

#aisymposium24

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SCS Swiss Chemical Society — Division of Fundamental Research

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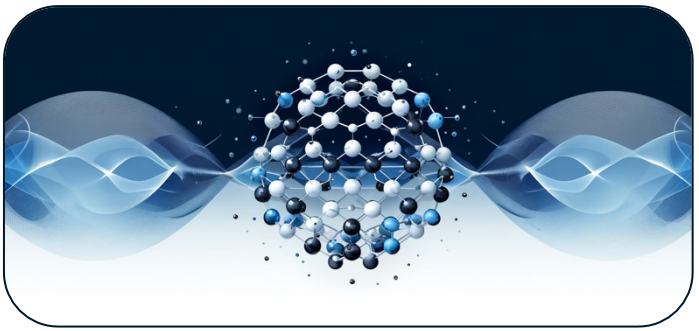
SCS Symposium on AI 2024

« Critical use of Artificial Intelligence in Chemistry »

University of Fribourg
November 25, 2024, 09.00 - 18.00



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Organizing Committee

Prof. Stefan Vučković, University of Fribourg (Chair)
Dr. Miroslava Nedyalkova, University of Fribourg
Dr. Attila Cangi, Helmholtz-Zentrum Dresden-Rossendorf

Registration

Participation is free of charge. However, registration is mandatory via the conference website: *https://ai24.scg.ch/registration*

Deadlines

Fri, 04.11.2024	Deadline poster application (call for abstracts)
Wed, 15.11.2024	Notification of acceptance for posters and the two contributed talks
Fri, 16.11.2024	Deadline for registration
Mon, 25.11.2024	Start of the event

Location

University of Fribourg
Department of Chemistry
Chemin du Musée 9
1700 Fribourg

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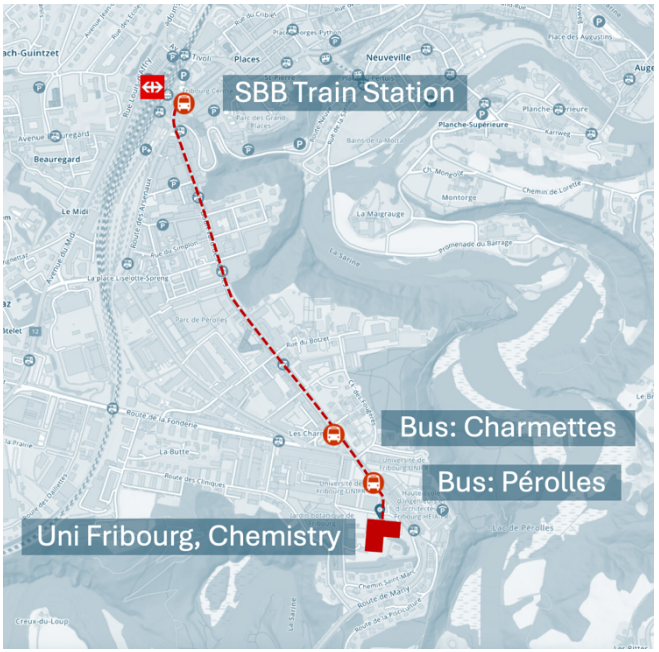

Program

09.00	Welcome Coffee and Registration
09.30	Welcome Message by ***Prof. Stefan Vuckovic***, University of Fribourg
09.45	***Prof. Sereina Riniker***, ETH Zurich «Learning physical interactions for molecular dynamics simulations»
10.25	***Dr. Ruben Laplaza***, EPFL Lausanne «Navigating homogeneous catalyst landscapes»
11.05	Short break
11.25	2 contributed talks à 15min Application deadline is November 11
11.55	***Dr. Zoe Cournia***, Biomedical Research Foundation Academy of Athens> «Predicting protein-ligand, protein-protein and protein-membrane interactions using molecular simulations and AI»
12.35	Lunchbreak Poster Session
14.00	***Prof. Alexandre Tkatchenko***, University of Luxembourg «Towards AI-enabled Fully Quantum (Bio)Molecular Simulations»
14.40	***Dr. Elias Polak***, University of Fribourg «Real-space machine learning of correlation density functionals»
15.20	Short break
15.40	***Prof. Jeremy Richardson***, ETH Zurich «Machine-learning acceleration for semiclassical and nonadiabatic dynamics»
16.20	***Prof. Markus Meuwly***, University of Basel «Constructing, Validating and Using Machine-Learned Potential Energy Surfaces»
17.10	Closing words
17.15	Aperitif
18.00	End of the Symposium

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