Università degli Studi di Padova

DiSC

Monday **30th September 2024** at **15:00** in room F of DiSC

Prof. Dr. Pascal Friederich

Department of Informatics & Institute of Nanotechnology,
Karlsruhe Institute of Technology

will give a talk entitled:

Machine Learning for Design, Understanding, and Discovery of Molecules and Materials

Machine learning can accelerate the screening, design and discovery of new molecules and materials in multiple ways, e.g. by virtually predicting properties of molecules and materials, by extracting hidden relations from large amounts of simulated or experimental data, or even by interfacing machine learning algorithms for autonomous decision-making directly with automated high-throughput experiments. In this talk, I will focus on our research activities on graph neural networks for property prediction [1] and understanding of structure property relations [2], as well as on the use of machine learning for automated data analysis and autonomous decision-making in self-driving labs [3].

[1] Reiser et al., Communications Materials 3 (1) (2022), https://www.nature.com/articles/s43246-022-00315-6
[2] Teufel et al., MEGAN: Multi-Explanation Graph Attention Network (2023), https://arxiv.org/abs/2211.13236
[3] Wu et al., JACS 2023, https://pubs.acs.org/doi/full/10.1021/jacs.3c03271

Your presence will be much appreciated

Host
Prof. Vincenzo Amendola

Il Direttore del Dipartimento
Prof. Stefano Mammi

Short Biography:

After his B.S. and M.Sc. in physics and a Ph.D. in physics on multiscale modeling of organic semiconductors, Pascal Friederich received a Marie-Sklodowska-Curie Postdoctoral Fellowship at Harvard University and the University of Toronto where he worked on machine learning methods for chemistry. In 2020, Pascal Friederich joined the Informatics Department of the Karlsruhe Institute of Technology as a tenure-track professor, leading the AI for Materials Science (AiMat, https://aimat.science) research group. The AiMat research group focuses on developing and applying machine learning methods for property prediction, simulation, understanding, and design of molecules and materials, as well as on interfacing machine learning methods with automated materials experiments. In 2022, Pascal Friederich received the Heinz-Maier-Leibnitz Prize from the German Research Foundation.