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S E M I N A I R E

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« Trusted AI for Accelerating Scientific Discovery »

Scientific discovery is one of primary factors underlying advancement of human race. However, traditional discovery process is slow compared to the growing need of new inventions. Machine learning and especially deep learning have achieved remarkable performance in domains like computer vision and natural language processing in recent years. Those methods have also infiltrated physics, chemistry, and medicine. Despite several successes and the potential, machine learning models are still at infancy in terms of driving and transforming scientific discovery. In this talk, I will present a closed-loop paradigm to accelerate scientific discovery, which can seamlessly integrate machine learning, physics-based simulations, and wet lab experiments and enable new hypothesis and/or artefact generation and validation thereof. Development and use of novel generative AI models, combined with further learning and optimization methods, for designing novel antimicrobials, drug candidates, and metamaterials with desired functionality will be discussed. Finally, I will discuss the importance of adding crucial aspects, e.g. creativity, robustness, and interpretability, to infuse elements of trust in machine learning models in order to enable and add value to AI-driven discovery.

Wednesday 13 January at 4pm CEST