IMCN SEMINAR

« Deep learning for materials design, drug discovery, and beyond »

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Auditorium Jean-Baptiste CARNOY (B.059)
Croix du Sud 4, Louvain-La-Neuve

More information: Sophie HERMANS (sophie.hermans@uclouvain.be)
Gian-Marco RIGNANESE (gian-marco.Rignanese@uclouvain.be)
ABSTRACT

We present a deep learning tool that merges all possible sources of information: computer simulations, physical laws, hidden variables, and even noise. The tool can exploit all possible sources of information to make the best possible predictions. We illustrate the tool through case studies that include experimental validation and have all led to commercialization: we design a nickel-base alloy for direct laser deposition from a training set containing just ten core results by juxtaposing complementary material properties; a molybdenum-base alloy for a forging hammer; a smallmolecule bioactivity database was initially 0.05% complete is imputed to be 30% complete, which is then used to design new drugs; and we present further examples spanning healthcare to infrastructure.

BIOGRAPHY

Gareth Conduit has a track record of applying artificial intelligence to solve real-world problems. The approach, originally developed for materials design, is now being commercialized by startup Intellegens in not only materials design, but also infrastructure, drug discovery, and healthcare. Previously, Gareth had research interests in strongly correlated phenomena, in particular proposing spin spiral state in the itinerant ferromagnet that was later observed in CeFePO; and studying the few-body to many-body crossover that inspired ultra cold atom gas experiment. Gareth’s group is based at the University of Cambridge.

Website: https://www.tcm.phy.cam.ac.uk/profiles/gjc29/