University of Twente, Enschede
Friday, 22 April 2022

Focus session ‘Machine learning and materials’

(An explanation in Dutch follows the abstracts)

Program:

- Hans Hilgenkamp (UT): Introduction to the Focus Session 'Machine Learning and Materials'
- Menno Bokdam (UT): Machine Learning Force Fields: unlocking the materials’ free energy
- Tamalika Banerjee (RUG): Complex-oxide based memristive devices for neuromorphic hardware
- Marjolein Dijkstra (UU): Machine learning soft materials
- Johan Mentink (RU): Machine learning ultrafast magnetism: access the inaccessible

Session organiser: Harold Zandvliet (UT)

Abstracts:

<u>Hans Hilgenkamp (UT): Introduction to the Focus Session 'Machine Learning and Materials'</u>

A brief introduction will be given to the topic of Machine Learning. From a physics and materials science view-point several aspects are of particular interest, like the use of machine learning in scientific discovery and the development of novel materials and device concepts for more (energy-)efficient machine learning applications. I will provide a brief overview on key challenges and developments, as a lead up to the other speakers of this session.

<u>Menno Bokdam (UT): Machine Learning Force Fields: unlocking the materials’ free energy</u>

Machine Learning has recently proven itself as the new “work horse” for atomic-scale condensed matter simulations under isothermal-isobaric conditions. Even though accurate predictions of internal energies of crystal structures from first principles based computational methods were available for many years, the materials’ free energy was (except for simple harmonic crystals) not accessible. I will highlight some of the latest ML developments and the opportunities they present.

<u>Tamalika Banerjee (RUG): Complex-oxide based memristive devices for neuromorphic hardware</u>

Most computers use the von Neumann architecture, where the separation between computation and storage limits power efficiency and component scalability. In contrast, a noteworthy feature of the human brain is that there is no clear separation between units that compute and store memory. Instead, these functions are accomplished by neurons and a large number of interconnections or synapses making them energy efficient. New paradigms are being researched where memory devices can be used both for storage and computation. In this context there is a renewed surge in different types of memristive devices, as hardware components for beyond von Neumann computation in which the resistance be controllably changed by an external stimulus, can exhibit multistate behavior for the same control parameter and information can be stored as conductance.

In this context we have exploited the rich phase space, intrinsic to complex oxides, for electronic property tunability, primarily of multistate resistance, by electric field and magnetization control. For this we design interface based memristive devices on unconventional oxide semiconductors, Nb doped $SrTiO_3$, using magnetic electrodes that act as analog synaptic weights and demonstrate multi-level switching between highly resistive states with resistance variations up to three orders of magnitude and read powers in the nW regime. From the SET behavior of the memristors, power-law learning models are developed and tested in a network consisting of Arduino nanos, mimicking tasks that cannot be addressed by a single perceptron. After training, this small network distinguishes horizontal and vertical lines with an accuracy of >90%, even with noisy input patterns. We have further extended the versatility of the memristive behavior by exploiting new approaches in spintronics using itinerant ferromagnetic oxides such as $SrRuO_3$. By controlling the magnetocrystalline anisotropy in these materials we show how a magnetic field can be used to access different non-volatile states in $SrRuO_3$ thin film devices with prospects for spin-orbit torque switching in engineered devices. Different approaches to control resistance states in an analog fashion, utilizing the versatility of complex oxides establishes these materials as promising building block for low power neuromorphic computing.

Marjolein Dijkstra (UU): Machine learning soft materials

Predicting the emergent properties of a material from a microscopic description is a scientific challenge. Machine learning has opened new paradigms in the understanding and design of materials. However, the soft-matter field has lagged far behind in embracing this approach for materials design. The main difficulty stems from the importance of entropy in soft-matter systems, which not only results in a highly complex phase behavior, but also in thermodynamic phases that are highly susceptible to thermal fluctuations. The abundance of exotic phases with (partial) orientation and positional order like liquid crystals, quasicrystals, plastic crystals, along with the omnipresent thermal noise, makes the classification of these states of matter using ML tools highly non-trivial. I will address questions like: Can we use machine learning to detect phase transitions, classify phases and find the corresponding order parameters, can we identify the kinetic pathways for phase transformations, and can we use machine learning to coarse-grain our models?

Johan Mentink (RU): Machine learning ultrafast magnetism: access the inaccessible

Although magnetism is one of the strongest quantum effects, many properties of magnetic materials in equilibrium are well understood within classical thermodynamics. However, much less is known about the dynamics of magnetism in space and time. In particular, on the characteristic time scale (femtosecond) and length scale (nanometer) of the intrinsic magnetic interactions, quantum effects can become crucial. Interestingly, understanding such dynamics is not only of fundamental interest but also exhibits great potential for applications owing to the demand for smaller, faster and more energy-efficient data processing and storage technology.

In this talk I will address fundamental physical limits for information technology and highlight the potential of magnetism to come orders of magnitude closer to these limits than is realized with state-of-the art technology. Next, I will address the challenges to simulate magnetism at these limits and introduce the recently established neural-network quantum states to address these challenges. To illustrate the potential this machine learning approach, I will present recent predictions on the space-time dynamics of the two-dimensional Heisenberg antiferromagnet. Interestingly, we discovered that at the shortest length and time scales the dynamics features *supermagnonic* propagation: spin correlations that propagate faster than the fastest group or phase velocity of the system. We identify that the origin stems from the quantum spin character of the spins, yielding a speed that is up to 40% higher in the most challenging regime for which S=1/2.

Inspired by these powerful yet energy-hungry predictions, I will conclude by presenting the first results of our collaborative efforts towards energy-efficient computing with machine learning. We quantify both the energy efficiency and latency of near-commercial in-memory computing hardware against standard CPU and GPU. By directly programming machine learning methods in neuromorphic hardware, we aim to disclose machine learning workloads that are more energy-efficient and therefore can yield access to currently inaccessible physics.

Machine learning and materials

In deze parallelsessie ligt het accent op het onderzoek aan neuromorfische materialen en op machine learning gebaseerde algoritmes die kunnen worden toegepast voor complexe berekeningen op dat gebied. Het is de bedoeling dat, gebruikmakend van deze neuromorfische materialen, in de toekomst krachtige, energie-efficiënte en fouttolerante computers worden ontwikkeld die geïnspireerd zijn op het functioneren van onze hersenen. Afgezien van deze ontwikkelingen in de hardware is er ook op het gebied van de software nog een flinke stap voorwaarts te maken. Denk bijvoorbeeld aan de ontwikkeling en optimalisatie van algoritmes gebaseerd op machine learning.

Marjolein Dijkstra van de Universiteit Utrecht zal een voordracht verzorgen op het gebied van algoritmes gebaseerd op machine learning. Dijkstra maakt gebruik van deze algoritmes voor het uitvoeren van complexe berekeningen aan colloïdale systemen. Tamalika Banerjee van de Rijksuniversiteit Groningen houdt zich onder andere bezig met nieuwe, op elektronspin gebaseerde memristors. De eigenschappen van deze memristordevices zijn aanpasbaar en wel op zo’n wijze dat ze in principe de werking van onze hersencellen kunnen nabootsen. De bedoeling is dat deze devices op de lange termijn zo krachtig en veelzijdig gaan worden dat ze de cognitieve taken van onze hersenen kunnen nabootsen. In haar voordracht zal Banerjee ingaan op de nieuwe ontwikkelingen in dit interessante vakgebied. Johan Mentink van de Radboud Universiteit in Nijmegen is expert op het gebied van de ultrasnelle dynamica in vaste stoffen, met name wat betreft de theoretische beschrijving en numerieke simulatie van quantum-many-body-effecten van de ultrasnelle dynamica in magnetische systemen. Hij houdt zich actief bezig met de toepassing van deze fenomenen voor de ontwikkeling van nieuwe concepten die het mogelijk maken om op een snellere, kleinere en meer energie-efficiënte wijze door het brein geïnspireerde berekeningen uit te kunnen voeren. In zijn voordracht zal Mentink uitvoerig ingaan op de ontwikkeling en mogelijke toepassingen van deze nieuwe concepten.

De sessie zal worden geleid en ingeleid door Hans Hilgenkamp en Menno Bokdam van de Universiteit Twente. Menno Bokdam is een onlangs aangestelde tenure tracker die o.a. actief is op het gebied van machine learning. Hans Hilgenkamp leidt samen met Wilfred van der Wiel het Center for Brain-Inspired Nano Systems (BRAINS) van de Universiteit Twente. Binnen dit centrum worden de expertises in nanoscience en nanotechnologie gecombineerd met die in computerwetenschap, kunstmatige intelligentie en neuroscience. Het doel is de ontwikkeling van een nieuwe generatie energie-efficiënte, op het brein geïnspireerde hardware voor een duurzamere informatietechnologie en voor toepassingen waarvoor oplossingen met gangbare elektronica niet optimaal zijn.

Harold Zandvliet is hoogleraar Technische Natuurkunde aan de Universiteit Twente. Hij houdt zich onder andere bezig met onderzoek aan 1D- en 2D-materialen.