Neuromorphic matter bottom-up constructed from individual atoms

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Summary. A physical realization of energy-based machine learning models relies on creating tunable multi-well energy landscapes. We have demonstrated a bottom-up platform, where orbital memory in Co and Fe atoms adsorbed on a black phosphorus surface can be manipulated to create such energy landscapes, using scanning tunneling microscopy. We show that the resultant dynamics of coupled arrays of orbital memory exhibit a physical realization of the famed Boltzmann machine. The system response is tunable by variation of atomic species and interatomic distances, as well as using varying input waveforms. Thus, this approach facilitates the design of materials with inherently neuromorphic properties on the atomic scale.

A crucial problem in neuromorphic computing is relating the computational characteristics of the brain to materials properties (*1*). In the current paradigm, machine learning algorithms are used as a starting point. Then, a subset of material properties, for example hysteresis or non-linearity, are used to build up complex circuitry that can mimic the chosen machine learning task. Yet, the similarities to the computational complexity of the brain are often limited. For example, in the brain, there is no distinction between hardware and software, contrary to conventional computing approaches. Moreover, aspects of the brain, such as self-learning and autonomous function are very difficult to implement in today's computing platforms. Implementing these aspects inherently in a material to carry out machine learning tasks without the need for additional conventional circuitry promises a paradigm shift in the field of neuromorphic computing.

One of the challenges in building materials for neuromorphic computing is linking the physical properties of materials to desired functionalities, such as plasticitity, and learning. To this end, energy-based machine learning models, such as the Hopfield model (*2*), and the Boltzmann machine (BM) (*3*), provide a natural link between reductionist machine learning models and materials that are governed by similar Hamiltonians. In these models, multi-well energy landscapes arising in coupled spin arrays function as attractor networks. For shallow energy wells, stochastic fluctuations between nearly degenerate states arise, that associate the energy landscape with a probability distribution of states (see Figure 1). Tunable interactions in the material can modify the energy landscape, leading to different observed probability distributions.

We employ a bottom-up approach to create multi-level energy landscapes by constructing arrays consisting of single magnetic atoms on a semiconductor substrate of black phosphorus (BP) using scanning tunneling microscopy (STM). This is based on the concept of orbital memory (*4*, *5*), where the orbital

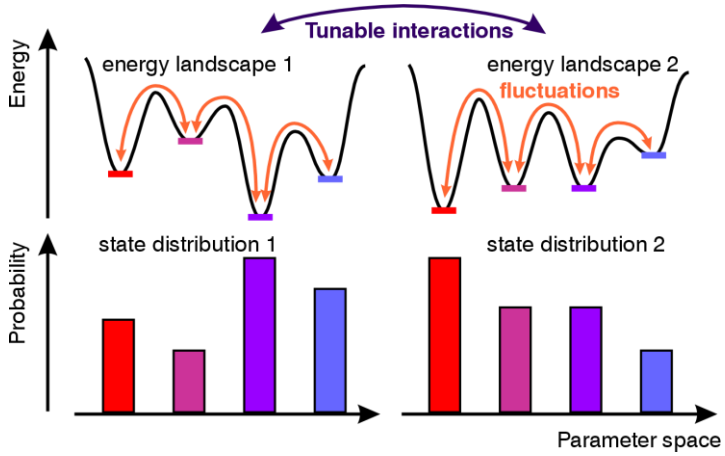

Figure 1. Two exemplary multi-well energy landscapes with stochastic fluctuations between energy minima and the corresponding probability distributions. Multi-well energy landscapes can be modified by tuning interactions in the material.

occupation exhibits bistability. Moreover, orbital memory can be tuned, via an external voltage, between a memory regime where a binary spin can be stored indefinitely, or into a stochastic regime, in which the binary spin fluctuates. Here, we present a model system where coupling orbital memory can be used to construct energy landscapes in analogy to the BM model. The construction atom-by-atom enables us to study and control the influence of geometry and interactions between spins on their stochastic dynamics.

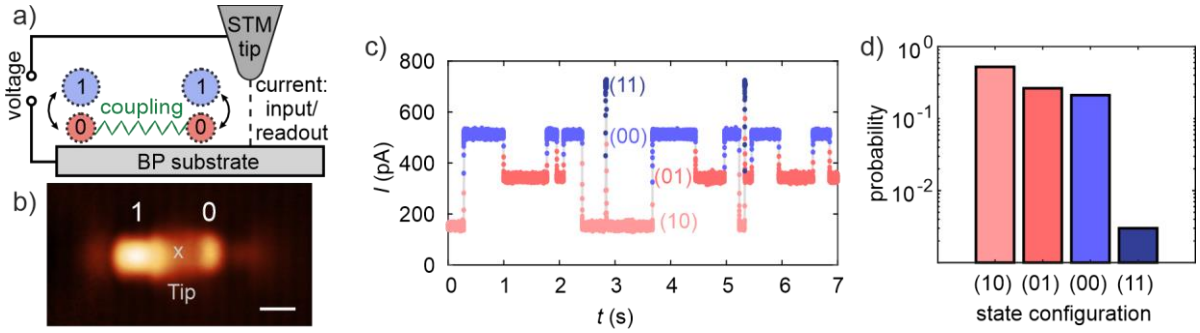

Figure 2. a) Schematic of bistable orbital memory in Co atoms on BP in an STM geometry. b) STM image of two Co atoms on BP in state "1" (left) and state "2" (right). Scalebar: 1 nm. c) Time trace and d) time-averaged state occupation of multi-level switching of the coupled Co atoms shown in b).

In this talk, the atomic BM will be reviewed, where we observe inherent plasticity and self-adaptation (*6*). Coupling strengths are governed by interatomic distances, which we have absolute control over. Figure 2a shows a sketch of our approach. The STM tip can be used to position the atoms on the BP substrate with sub-nanometer precision. By applying a voltage stimulus via the STM tip, stochastic switching of the atoms between orbital states "0" and "1" can be induced. The readout is done via detection of the state-sensitive tunnel current. An example of two coupled Co atoms in state (10) is given in Figure 2b. The x marks the tip position, where the current trace in (Figure 2c) was recorded. The probability distribution (Figure 2d) that characterizes the system can be deduced from the time-resolved data. It can be reconfigured by altering the coupling between individual atoms. We also review a more recent result, where local dopants can be used to locally gate individual spins in the energy landscape (*7*). The anisotropic nature of the BP substrate provides a means to realize dynamics on separate time scales: slowly changing variables alter the dynamics in the faster variables, which is a pathway to long-term potentiation. We will finally review new work on the stochastic dynamics in response to AC signals. These examples show that orbital memory provides a versatile way of realizing machine learning models in physical systems on the atomic scale. The small size at the fundamental atomic limit promises energy-efficiency and the semiconductor-based approach is advantageous in view of possible future integration in existing computation hardware.

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