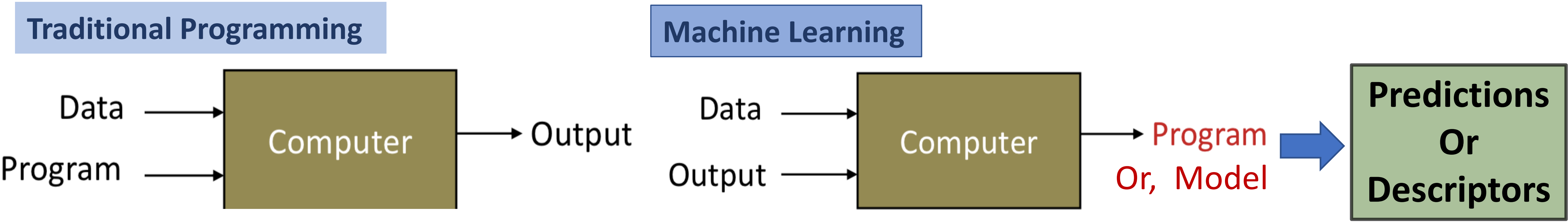
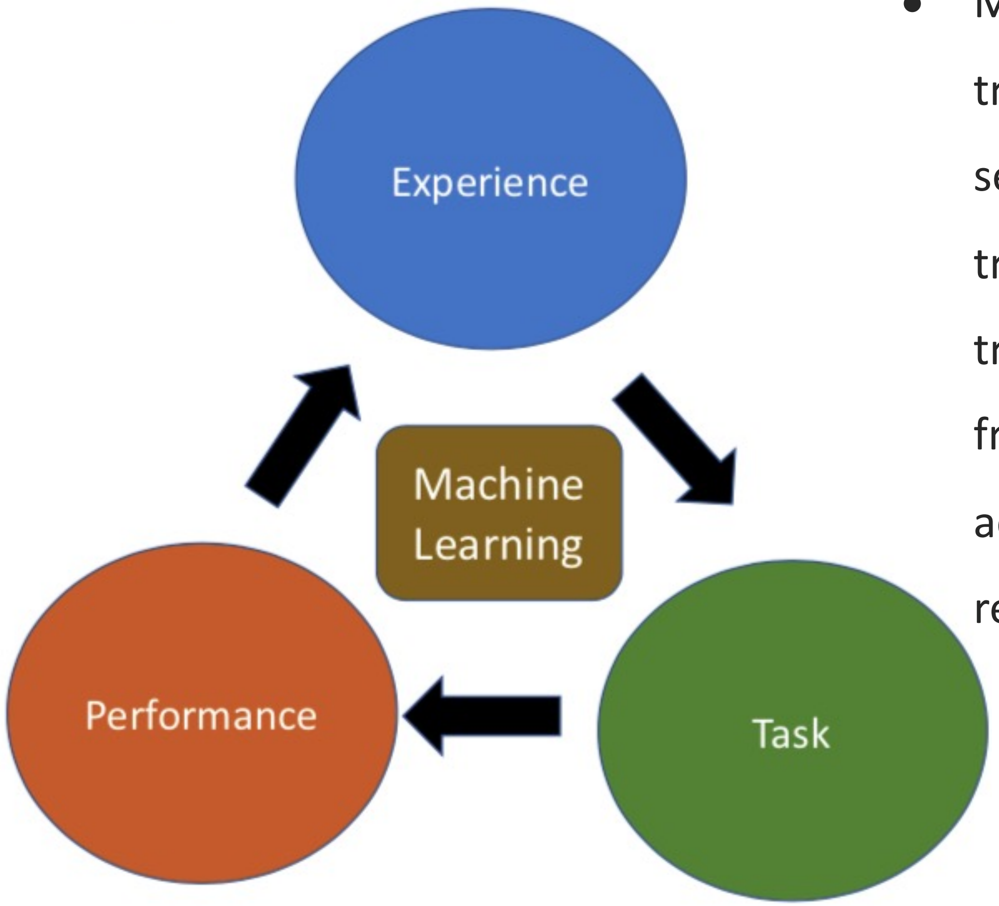
# Current computational and machine learning approach for as an electron microscopy image processing using Graphene

**What is machine learning? (Ref: https://mitsloan.mit.edu/ideas-made-to-matter/machine-learning-explained )**




- Machine learning (ML) is a subfield of artificial intelligence, which is broadly defined as the capability of a machine to imitate intelligent human behavior. Artificial intelligence (AI) systems are used to perform complex tasks in a way that is similar to how humans solve problems.
- The goal of AI is to create computer models that exhibit “intelligent behaviors” like humans, according to Boris Katz, a principal research scientist and head of the InfoLab Group at CSAIL. This means machines that can recognize a visual scene, understand a text written in natural language, or perform an action in the physical world.
- Machine learning is one way to use AI. It was defined in the 1950s by AI pioneer Arthur Samuel as “the field of study that gives computers the ability to learn without explicitly being programmed.”




- Machine learning starts with data — numbers, photos, or text, like bank transactions, pictures of people, repair records, time series data from sensors, or sales reports. The data is gathered and prepared to be used as training data, or the information the machine learning model will be trained on. The more data, the better the program. Some data is held out from the training data to be used as evaluation data, which tests how accurate the machine learning model is when it is shown new data. The result is a model that can be used in the future with different sets of data.

Machine learning working principle has been shown. The algorithms are design to work in three steps.

1. The computer has been asked to perform a task
2. The task performance will be evaluated, and a reward will be given
3. With the reward the computer will gain experience and finally with the experience gain it will perform the task again

This cycle will go on a training data and computer will build a model. Finally, the model will be tested in a training set for prediction and validation.

# Machine Learning in Materials Science

- **Supervised learning**
  - Prediction
  - Classification (discrete labels), Regression (real values)
- **Unsupervised learning**
  - Clustering
  - Probability distribution estimation
  - Finding association (in features)
  - Dimension reduction
- **Reinforcement learning**
  - Decision making (robot, chess machine)

**Supervised Learning**

**Dataset**: Has example inputs and outputs

**Objective**: Train a model to predict outputs from feature inputs.

**Classification**

The output variable is a category. e.g.

[spin up/spin down] or

[ferromagnetic/paramagnetic /diamagnetic]

**Regression**

Attempts to determine the relationship between one dependent variable and a series of independent variables.

**Unsupervised Learning**

**Dataset**: Only the inputs are known

**Objective**: Train a model to find existing patterns in the data to learn more about it.

**Association**

We want to discover rules that describes our data

e.g. material which is soluble in water, also soluble in kerosene.

**Clustering**

We want to discover the inherent categories in the data.

e.g. grouping of materials by their solubility.

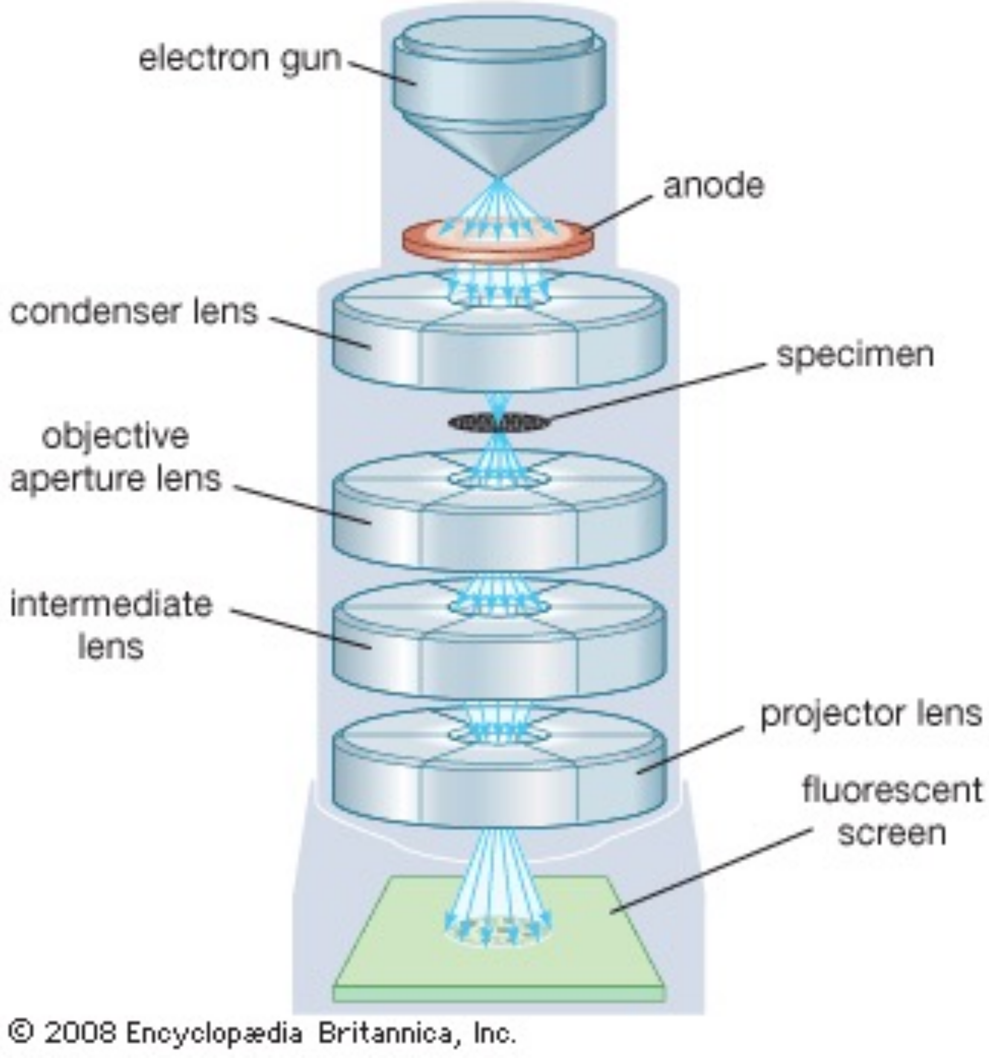
**Ref:** [1] Bishop CM. Pattern recognition and machine learning. New York: Springer; 2007.

- There are four types of machine learning that are commonly used in scientific fields
    - Unsupervised learning: In unsupervised learning, the agent learns patterns in the input, even when no explicit feedback is supplied. Clustering is a common example of an unsupervised task, which detects meaningful clusters among input data. For example, a regular office goer, Mr. Neogy, traveling from one area to the other in New York City, will develop a concept or percept of “good traffic days” and “bad traffic days” based on day to day experiences, without ever consulting motor vehicles department or traffic controllers for labelled examples of each.
- Supervised learning: In this mode, the agent learns from a function that maps the input output pairs from some observed instances present in the data. In Mr. Neogy’s case, inputs are percepts about traffic conditions that he has developed over time and outputs are provided by him, where he gives directions to the cab-driver. Besides the inputs provided by Mr. Neogy, here the cab-driver can also alter the outcome based on let’s say if he passes a bus or a car or a pedestrian on the road and decides to take a different route or more time. Now, Mr. Neogy’s final outcome of reaching office on time or late is a function of states such as his own perceptions as well as the cab driver’s actions like braking, accelerating or stopping distance. The output is directly available from the agent’s percepts, the cab-driver is the environment and the final outcome can be changed if either the percept or environment changes.

- Semi-supervised learning: In this mode, we are given a few labelled instances and a large set of unlabeled ones. Let's assume, we are given a task of creating a model to predict what type of coffee a person drinks on a regular basis. We can gather some data (labelled examples) by interviewing people and / or by visiting multiple coffee shops, which would be identical to supervised learning. However, in reality, some of the people interviewed may not be truthful in their responses. Furthermore, the collected data may be inaccurate for other reasons, e.g., people not knowing specific coffee types and naming different coffee brands instead. Therefore, there is not only random noise in the data, but there are systematic inaccuracies present that can only be identified by utilizing unsupervised learning techniques. In other words, noise and lack of labelled instances create a continuum between supervised and unsupervised learning modes, which constitutes the domain of applicability of semi-supervised approaches.

- Reinforcement learning: This is another hybrid mode in which the agent learns from a series of past events or reinforcements (success or failure). Here, the model gets either rewards or penalties for the actions it performs, such as searches or trials, with a goal to maximize the total reward. For example, if Mr. Neogy reaches his office on time, that gives him an indication that he did something right along the way. It then falls on the agent to decide which of the actions prior to reinforcement had the most pronounced impact on the outcome.

## What is electron microscopy? (Ref: https://www.thermofisher.com/us/en/home/materials-science/learning-center/applications/sem-tem-difference.html )




- Electron microscopes were developed in the 1930s to enable us to look more closely at objects than is possible with a light microscope. Scientists correctly predicted that a microscope that used electrons instead of visible light as the illumination source could view objects at far higher resolution than a light microscope. This is because the wavelength of visible light is what limits the resolution of light microscopes, and the wavelength of electrons is far smaller.

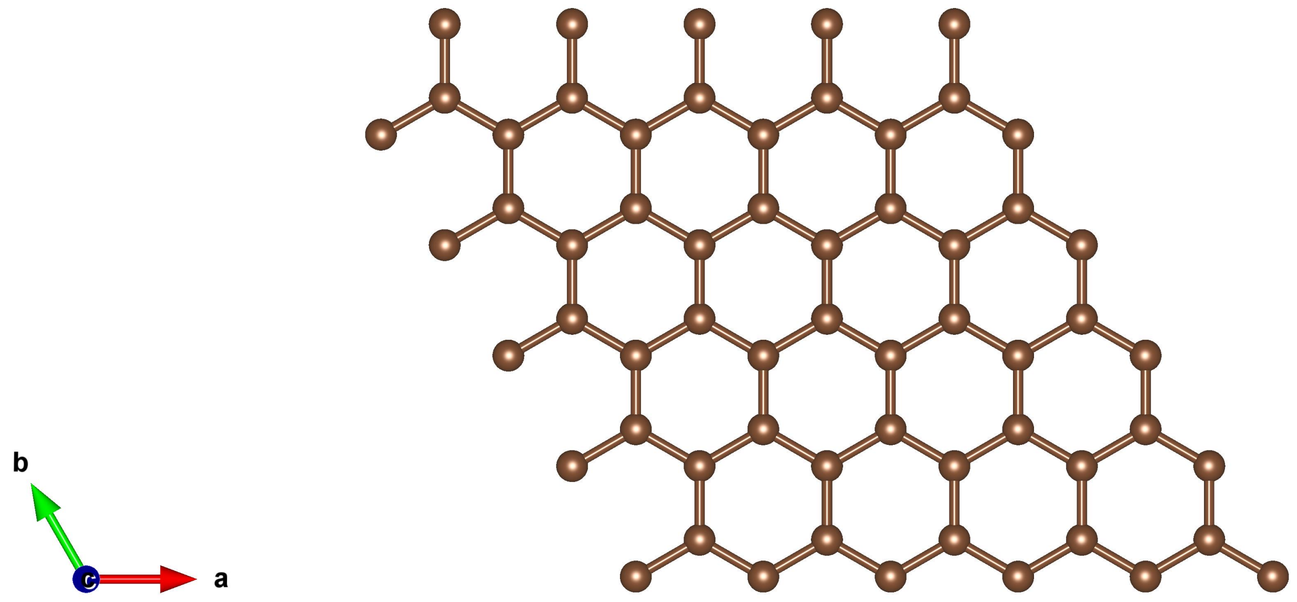
  - Electron microscopes use a beam of electrons rather than visible light to illuminate the sample.

- Some electron microscopes can detect objects that are approximately one-twentieth of a nanometer (10-9 m) in size – they can be used to visualize objects as small as viruses, molecules or even individual atoms.
- Electron microscopes have emerged as a powerful tool for the characterization of a wide range of materials. Their versatility and extremely high spatial resolution render them a very valuable tool for many applications. The two main types of electron microscopes are the transmission electron microscope (TEM) and the scanning electron microscope (SEM).
- The main difference between SEM and TEM is that SEM creates an image by detecting reflected or knocked-off electrons, while TEM uses transmitted electrons (electrons that are passing through the sample) to create an image. As a result, TEM offers valuable information on the inner structure of the sample, such as crystal structure, morphology and stress state information, while SEM provides information on the sample's surface and its composition.

- For both techniques, electrons are used to acquire images of samples. Their main components are the same:
    - An electron source
    - A series of electromagnetic and electrostatic lenses to control the shape and trajectory of the electron beam
    - Electron apertures
- All of these components are housed inside a chamber that is under high vacuum.

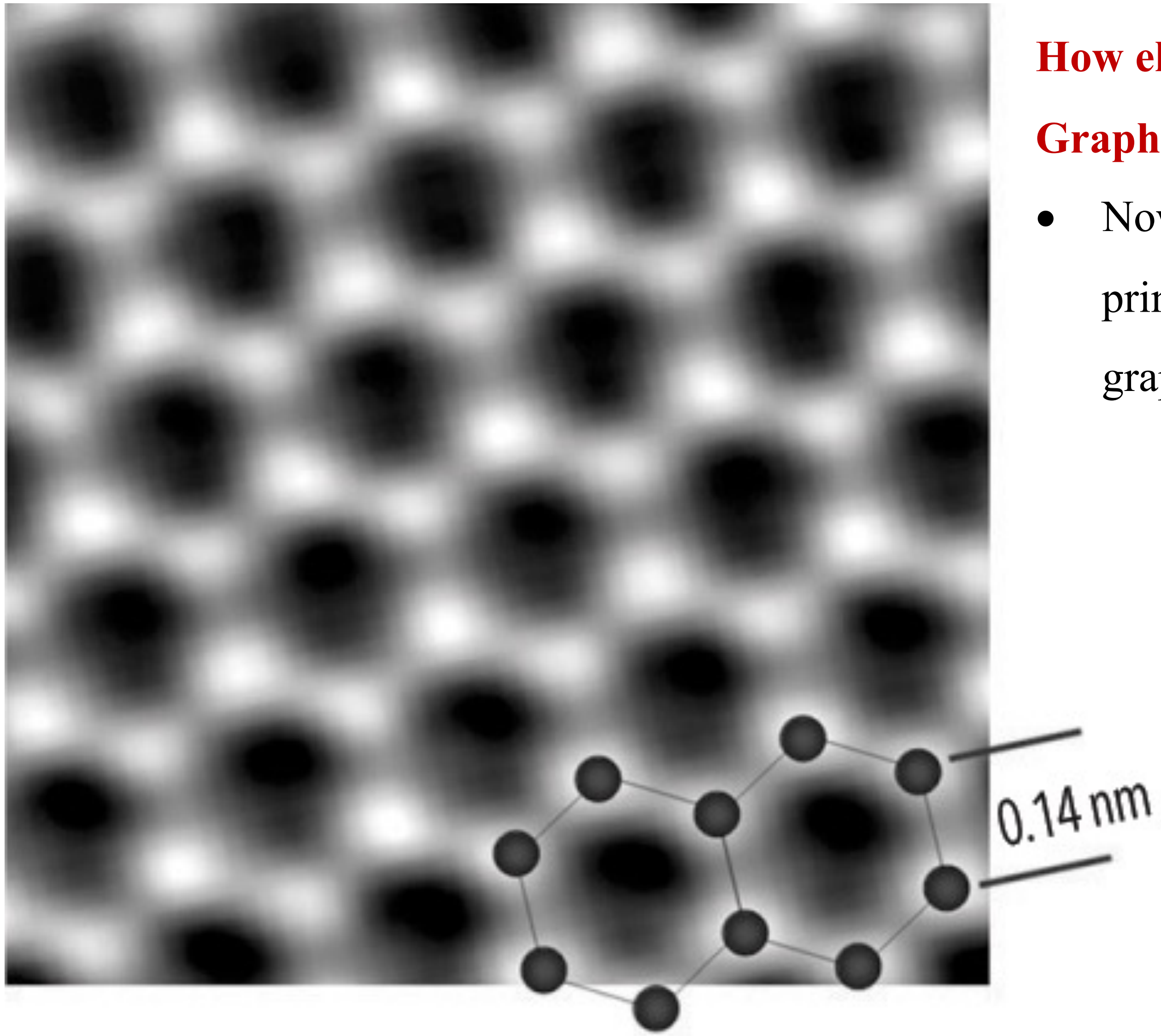
## What is a 2D material for example Graphene ?

Graphene is a single atomic layer of carbon atoms tightly packed in a two-dimensional honeycomb lattice. This novel material is atomically thin, chemically inert, consists of light atoms, and possesses a highly ordered structure. Graphene is electrically and thermally conductive, and is the strongest material ever measured. These remarkable properties make graphene the ideal support film for electron microscopy.



## How electron microscopy can be used to take images of a 2D Graphene

- Now that we know about SEM, TEM and STEM, their working principles, we can use either of the techniques to image a 2D graphene

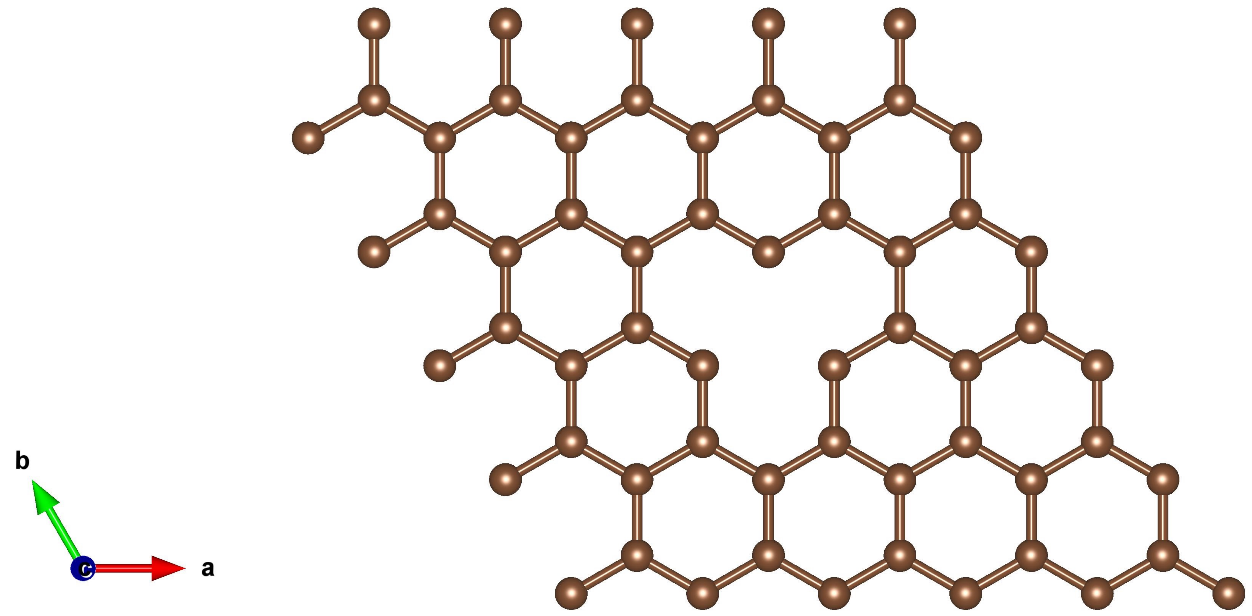



**Electron Microscope Image of a 2D material Graphene**

## What is the main challenge in electron microscopy of 2D Graphene?

Although the general structure of hexagonal rings of carbon can be seen by high-resolution microscopes, imaging the individual atoms and measuring their positions is not as straightforward.

The electron tip must scan the surface of the Graphene to take an electron microscope image. This way if the graphene surface is exposed to the electron beam for longer time, then defects will be formed in the Graphene.



## How can machine learning help?

The machine learning models build from a previous large data set  (taken from previous experiments) can help to guide on the (key points but not limited to)

(a) Explore time of the beam  to reduce defect formation
(b) Where is focus for a clean high-resolution image
(c) Improving signal-to-noise ratio, meaning increasing detections limits
(d) Finite control over the experimental procedure to reduce the human error during performance of the experiment.

## References


- Scanning Transmission Electron Microscopy Imaging and Analysis by Stephen J. Pennycook, Peter D. Nellist