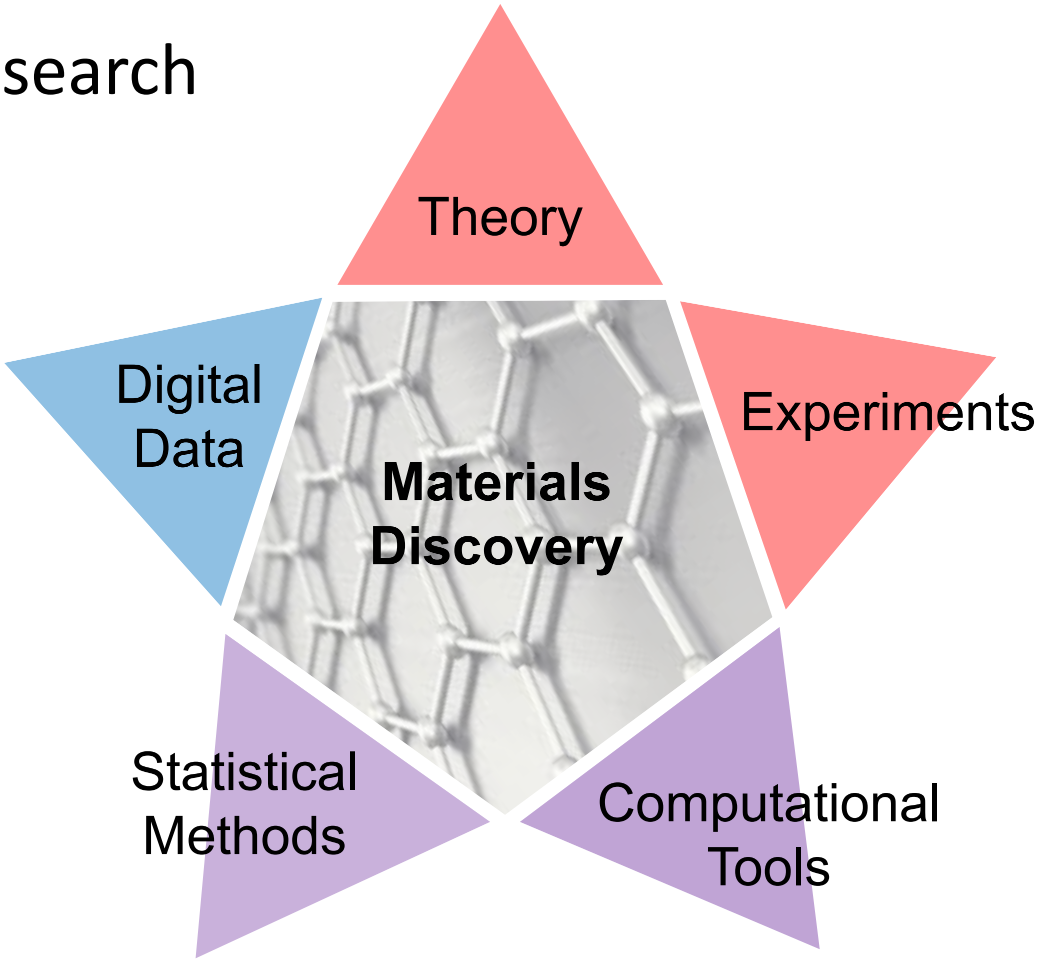
Machine Learning in Materials Physics Education

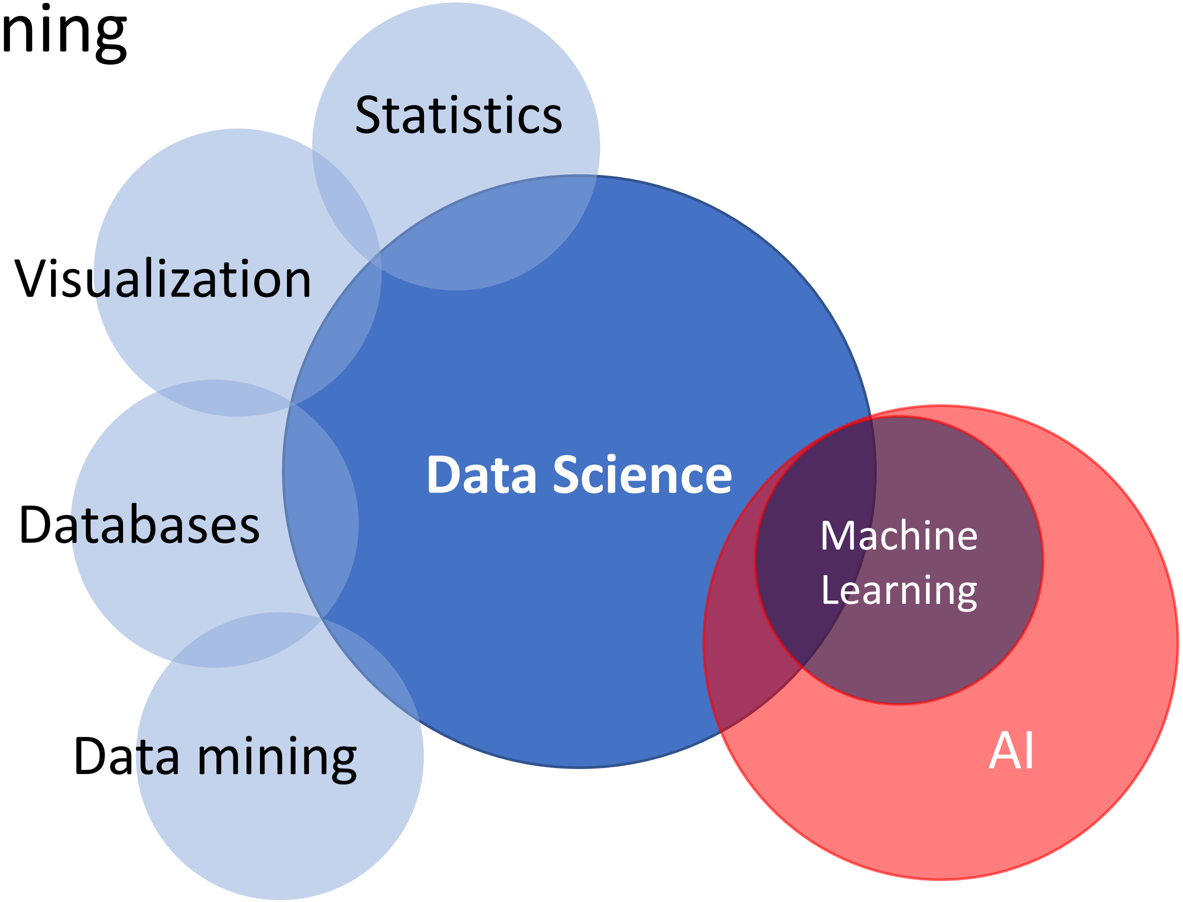
Trevor David Rhone

[1]Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute;

Materials research using ML



Machine learning



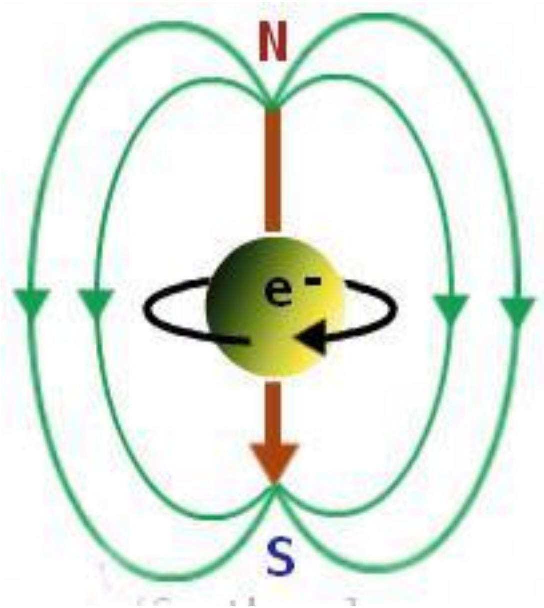
4 August 1972, Volume 177, Number 4047

SCIENCE

More Is Different

Broken symmetry and the nature of the hierarchical structure of science.

P. W. Anderson



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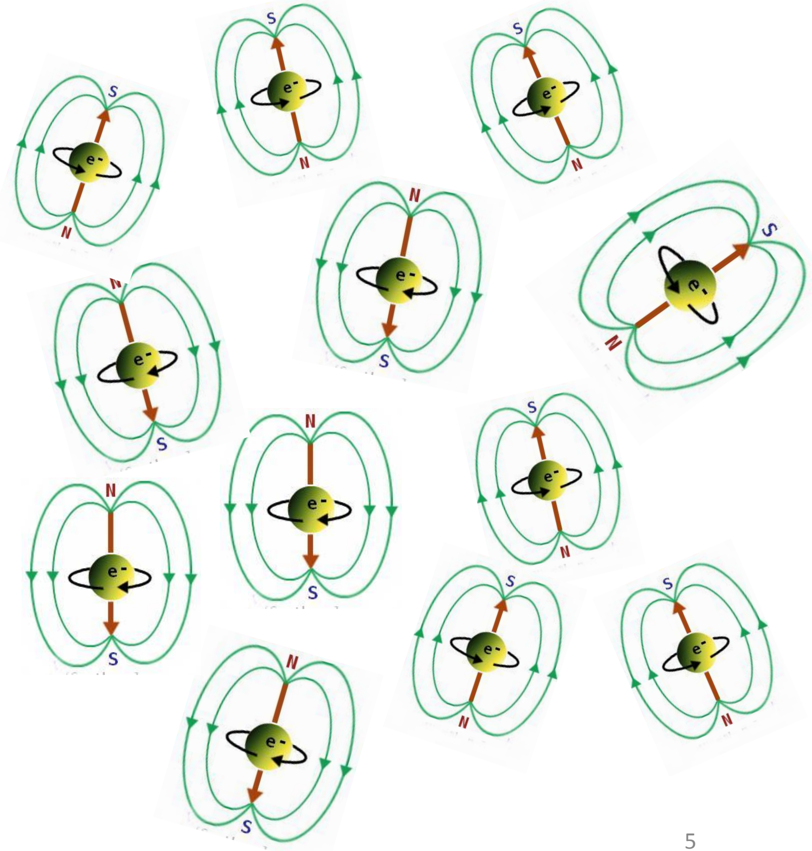
SCIENCE



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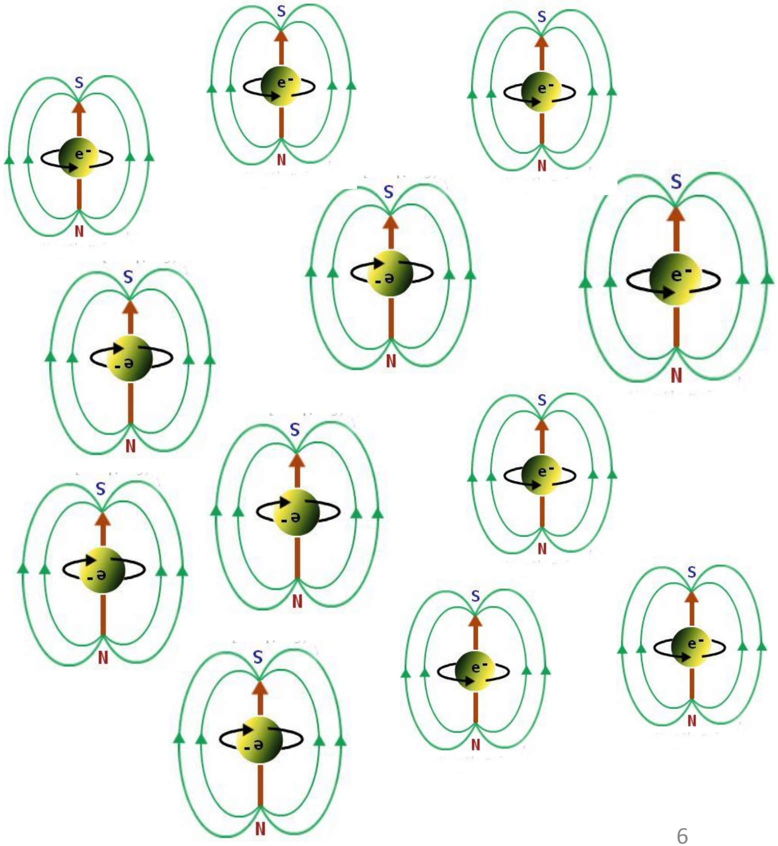
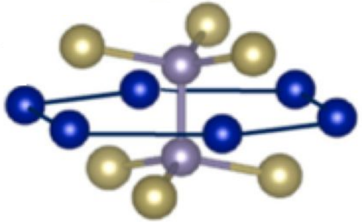
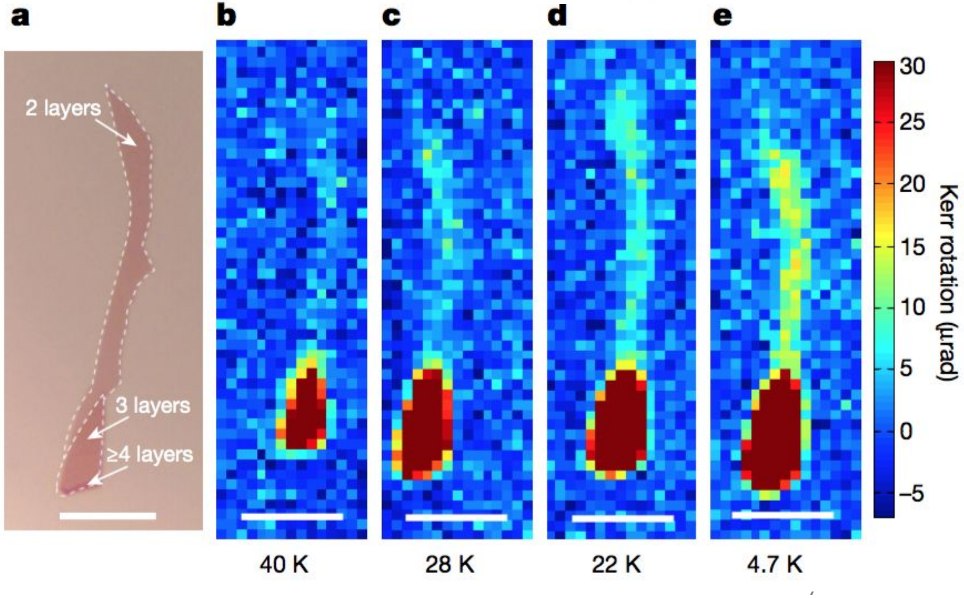


Magnetic two-dimensional materials

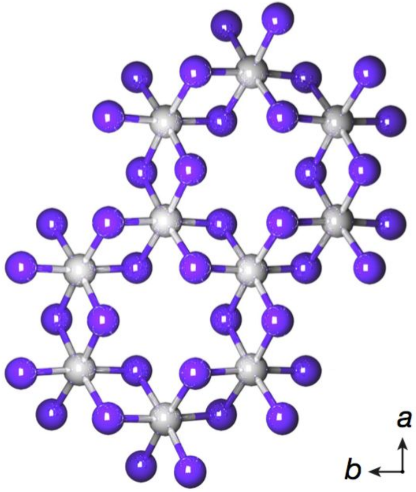
$Cr_2Ge_2Te_6$

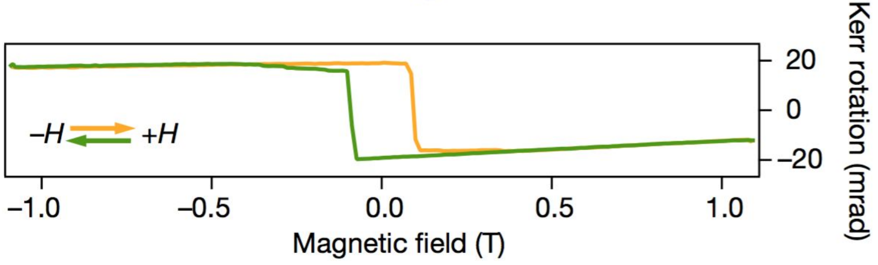




Gong, doi:10.1038/nature22060

CrI_3





Jarillo-Herrero,

Key Advances in Spin-Transfer-Torque MRAM

Device

1974

Slonczewski (IBM) invents magnetic tunnel junction.

1995

Moodera (MIT) and Miyazaki (Tohoku U.) demonstrate first room temperature magnetic tunnel junctions.

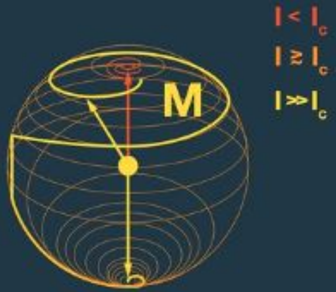
LOW RESISTANCE HIGH RESISTANCE

A magnetic tunnel junction is a sandwich of two magnetic layers separated by a thin insulating layer. When the two magnets both point in the same direction ('0' state), the resistance is low. When they point in opposite directions ('1' state), the resistance is high.

Write

1996

Slonczewski (IBM) invents spin-transfer-torque switching.



Spin torque switching is used to write the tunnel junction. As current is driven through the junction, the spins of the electrons are transferred from one magnet to the other magnet, thus switching it from pointing north to pointing south, or vice versa.

Read

2004

Parkin (IBM) and Yuasa (AIST) publish discovery of high magneto-resistance in MgO tunnel junctions.

The first junctions used amorphous AlOx tunnel barriers, but the change in resistance between '0' and '1' states was fairly small. Crystalline MgO tunnel barriers give much larger changes in resistance, typically about 2-3x, enabling faster read.

Scaling

2010

Worledge (IBM) and Ohno (Tohoku U.) demonstrate first perpendicular CoFeB tunnel junctions.

All early junctions had the north- south poles of the magnets lying in the plane of the wafer, even though Slonczewski had predicted having them aligned perpendicular to the plane of the wafer would require much lower write currents. New perpendicular magnetic materials had to be discovered to make this possible.

Infographic by StoryTK for IBM Research

ML in materials physics education

Overview

1. Physics research: Beginners guide to ML
2. Coursework: ML in physics
3. Workshops: Data science for physicists

- Machine learning for materials discovery
  - Two-dimensional (2D) magnetic materials

ML in materials physics education

Overview

1. Physics research: Beginners guide to ML
2. Coursework: ML in physics
3. Workshops: Data science for physicists

Magnetic two-dimensional materials

How do we find new 2D materials?

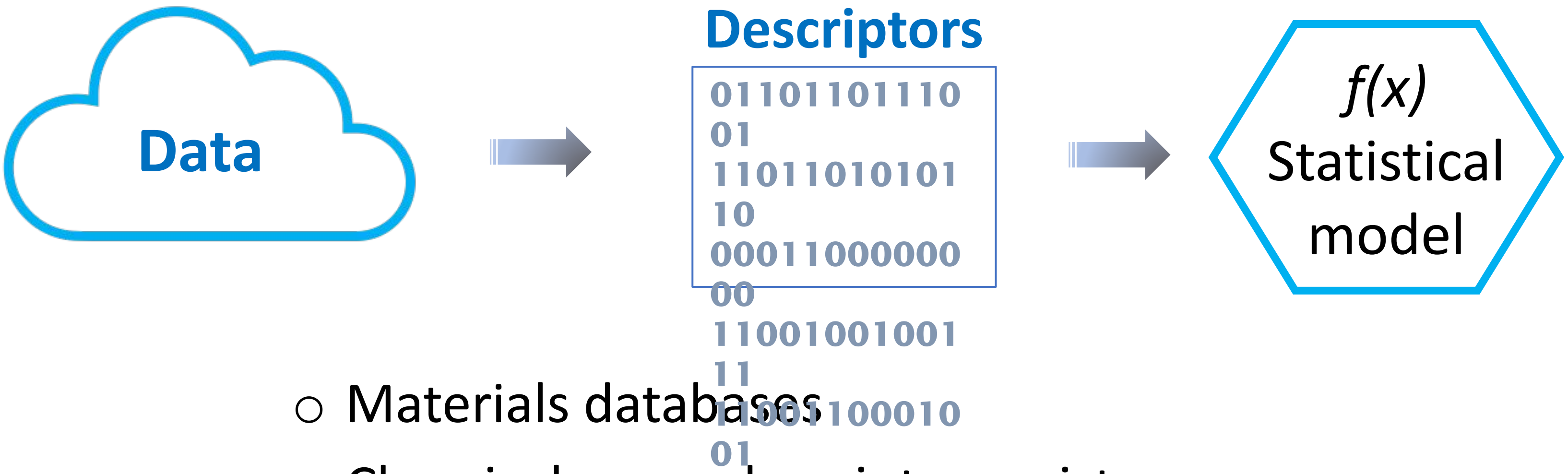
How to find new 2D magnetic materials?

Data-driven study of 2D magnetic materials

Materials science + Artificial intelligence

$$\underbrace{y}_{\substack{\text{Magnetic} \\ \text{moment}}} = \underbrace{f(x_1, x_2, \ldots, x_N)}_{\substack{\text{Number of spin up electrons} \\ \text{Number of valence electrons} \\ \ldots \\ \text{Electronegativity}}}$$

Machine Learning for Materials studies



- Materials databases
- Chemical space descriptors exist
- Datascience tools
    - Scikit learn, TensorFlow, Pytorch

Machine Learning for Materials studies

MATERIALSCLOUD

scientific reports

Data-driven studies of magnetic two-dimensional materials

Trevor David Rhone, Wei Chen, Shaan Desai, Steven B. Torrisi, Daniel T. Larson, Amir Yacoby & Efthimios Kaxiras

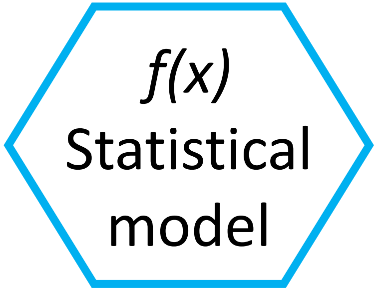
Machine Learning for Materials studies

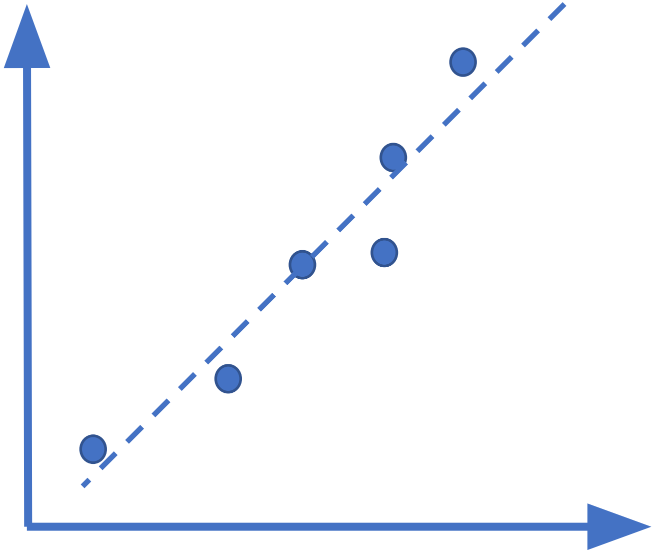
Descriptors

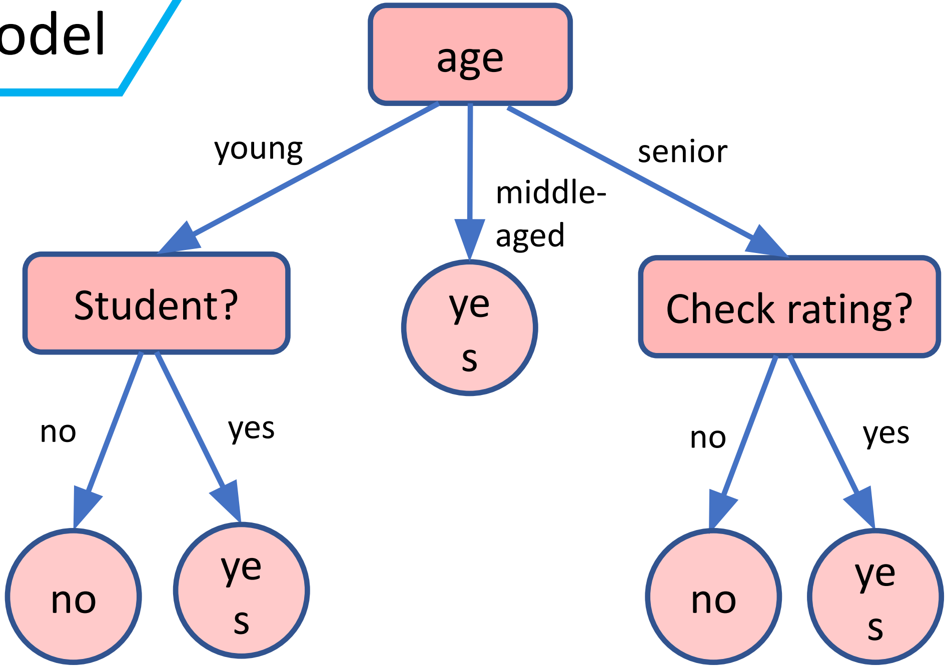
01101101110
01
11011010101
10
00011000000
00
11001001001
11
11001100010
01

- Mathematical representation of a material
  - Atomic properties
    - Pymatgen, Matminer
  - Encodes the crystal structure
    - SOAP kernal, Coulomb kernel (Dscribe python package)

Machine Learning for Materials studies







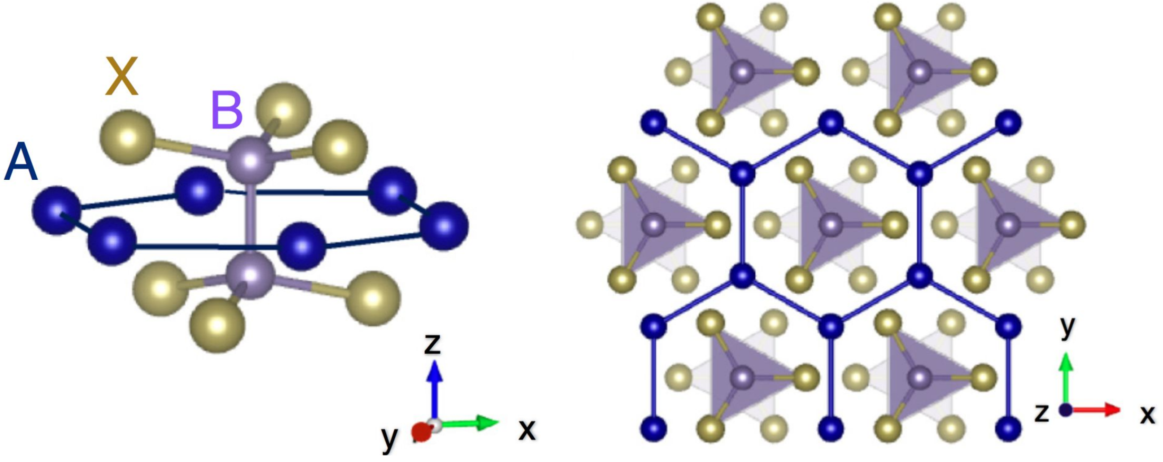
Machine Learning for Materials studies

Magnetic 2D crystals

Machine Learning for Materials studies

Magnetic 2D crystals

Transition metal chalcogenides are magnetic 2D crystals



$A_2B_2X_6$ crystal structure

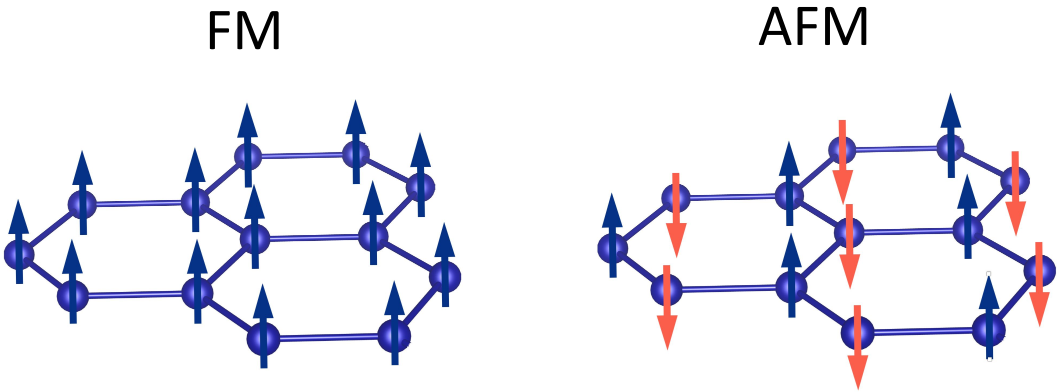
- $CrGeTe_3$ is a ferromagnet (FM)[1,2]
- $CrSiTe_3$ is an antiferromagnet (AFM)[1]

1. Sivadas et al., PRB 91 235425 (2015) 2. C. Gong et al., *Nature* **546**, 265 (2017)

Machine Learning for Materials studies

Magnetic 2D crystals

Transition metal chalcogenides are magnetic 2D crystals



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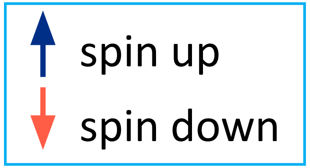
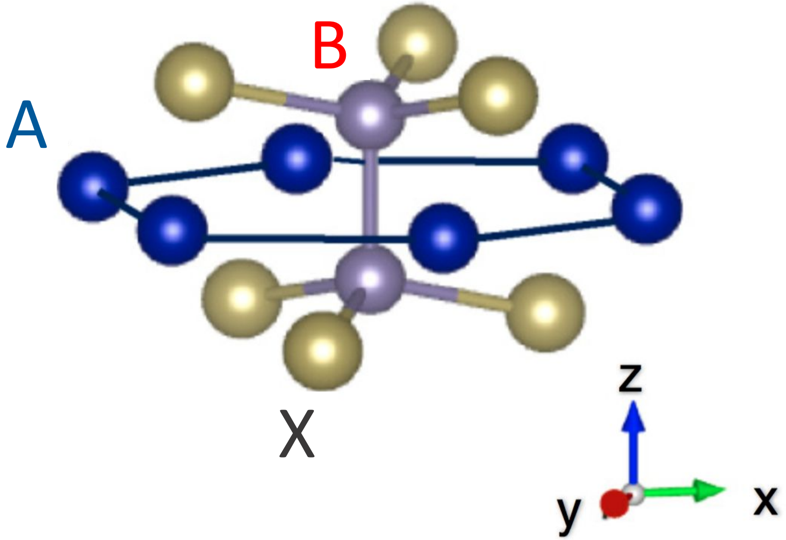


Magnetic configurations

1. Sivadas et al., PRB 91 235425 (2015) 2. C. Gong et al., *Nature* **546**, 265 (2017)

Magnetic van der Waals materials
$A_2B_2X_6$ structures

- 198 $A_2B_2X_6$ structures using first-principles quantum calculations (DFT)
  - Total # of structures $\sim 10^4$
  - NM, FM and AFM spin configurations
- Extract data:
  - Formation energy
  - Magnetic order
  - Magnetic moment

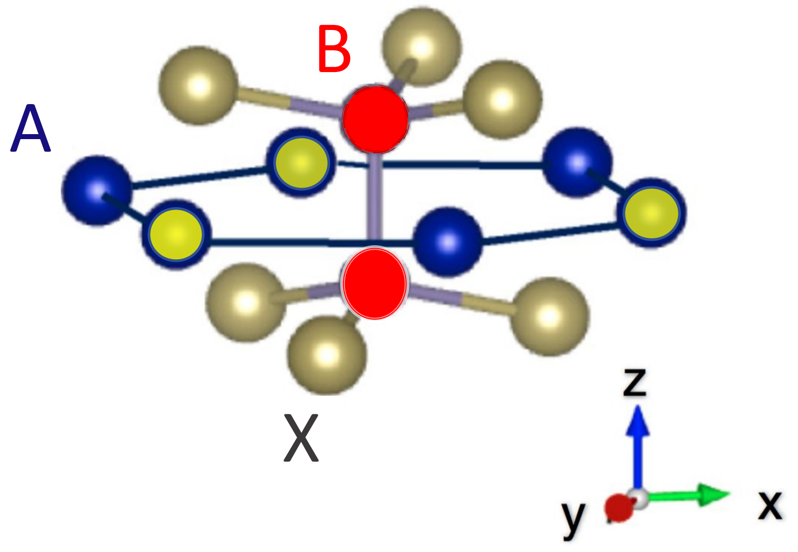


Rhone, T.D., *et al.*, *Sci Rep* **10,** 15795 (2020).

Magnetic van der Waals materials
$A_2B_2X_6$ structures

Substitutions:

- A site:
  - $Cr_{0.5}A_{0.5}$
  - A: Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Y, Nb, Ru
- B site:
  - Si, Ge, P combinations
  - B: Si, Ge, P, $Si_{0.5}Ge_{0.5}$, $Si_{0.5}P_{0.5}$, $Ge_{0.5}P_{0.5}$
- X site:
  - S, Se, Te



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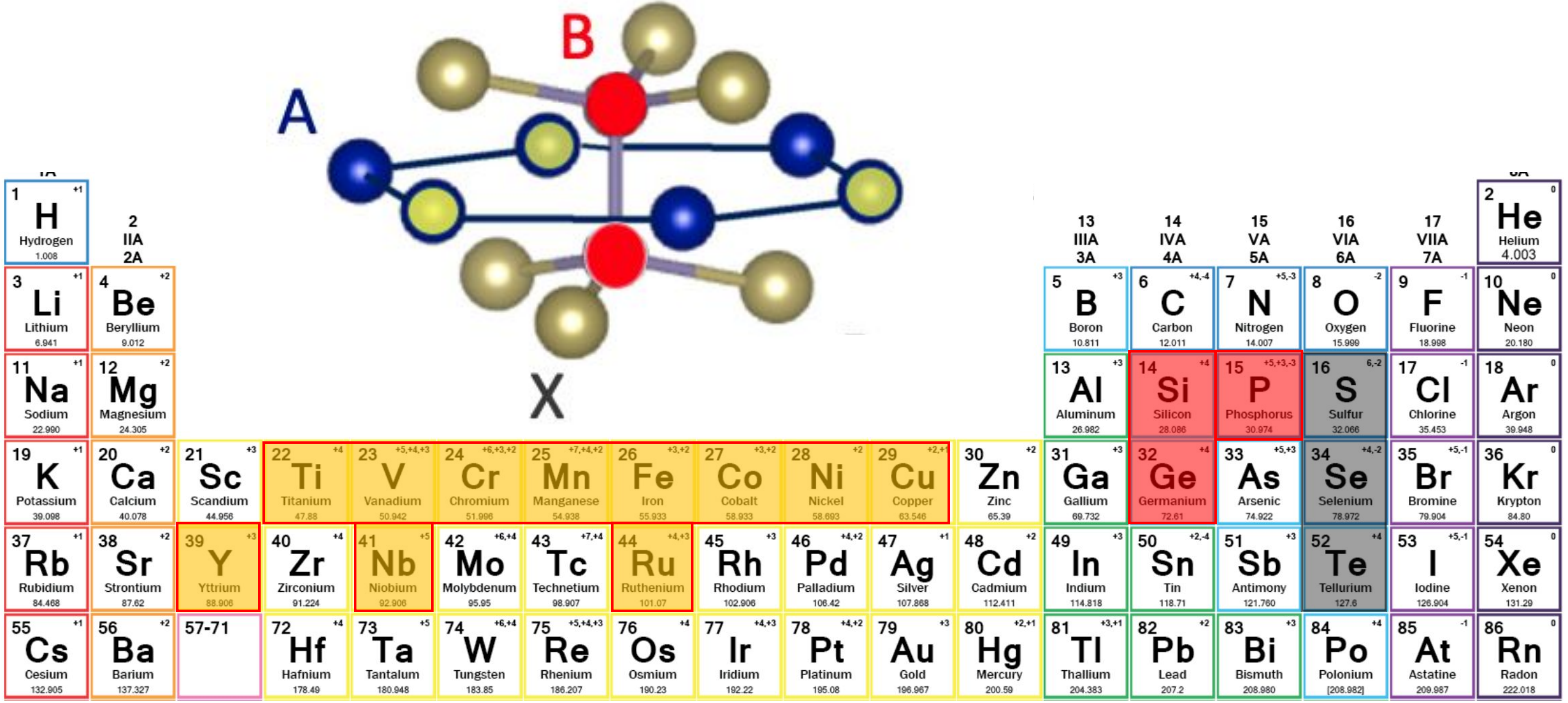
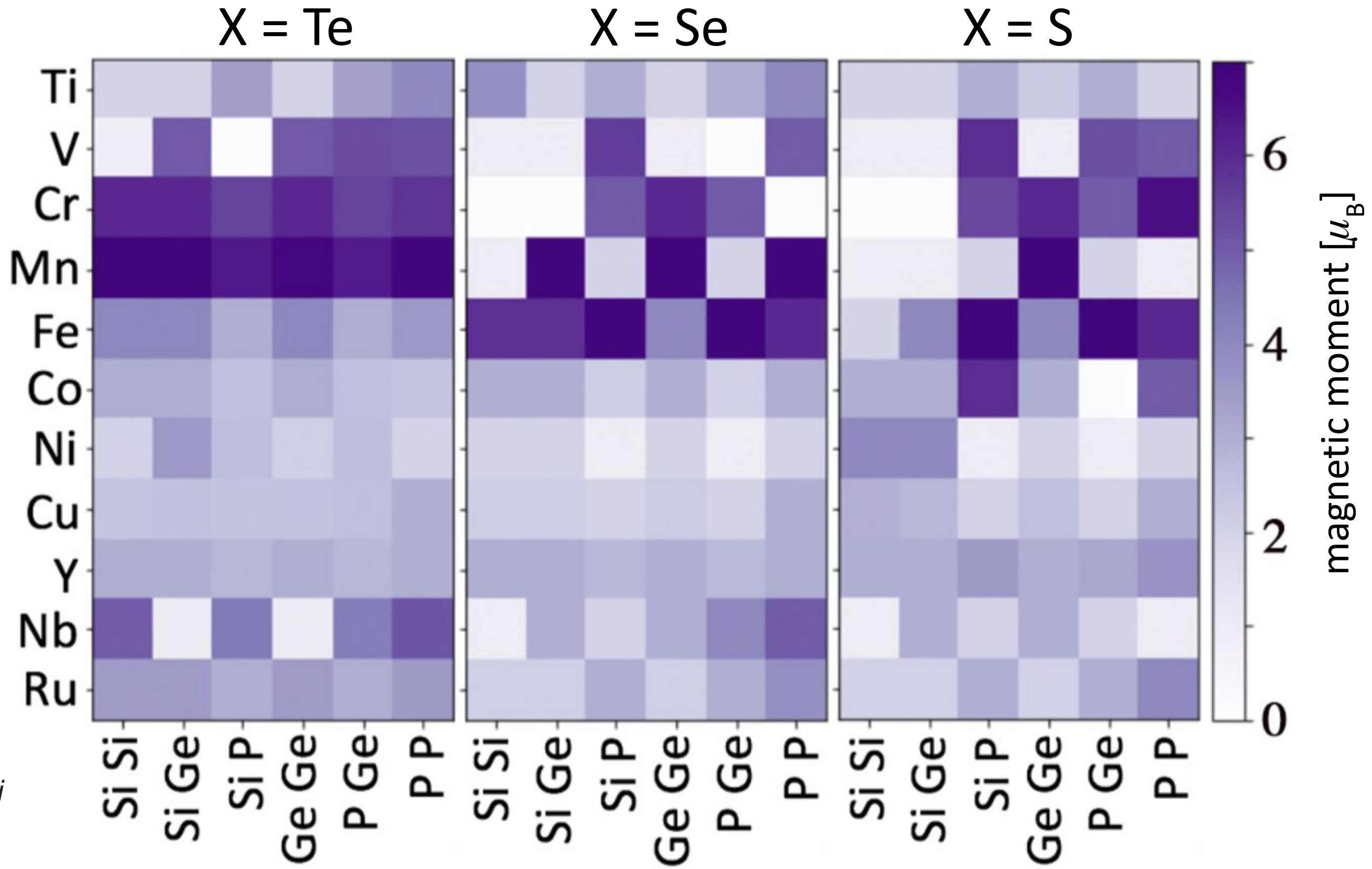
Magnetic van der Waals materials

$A_2B_2X_6$ structures



Magnetic moment of $A_2B_2X_6$

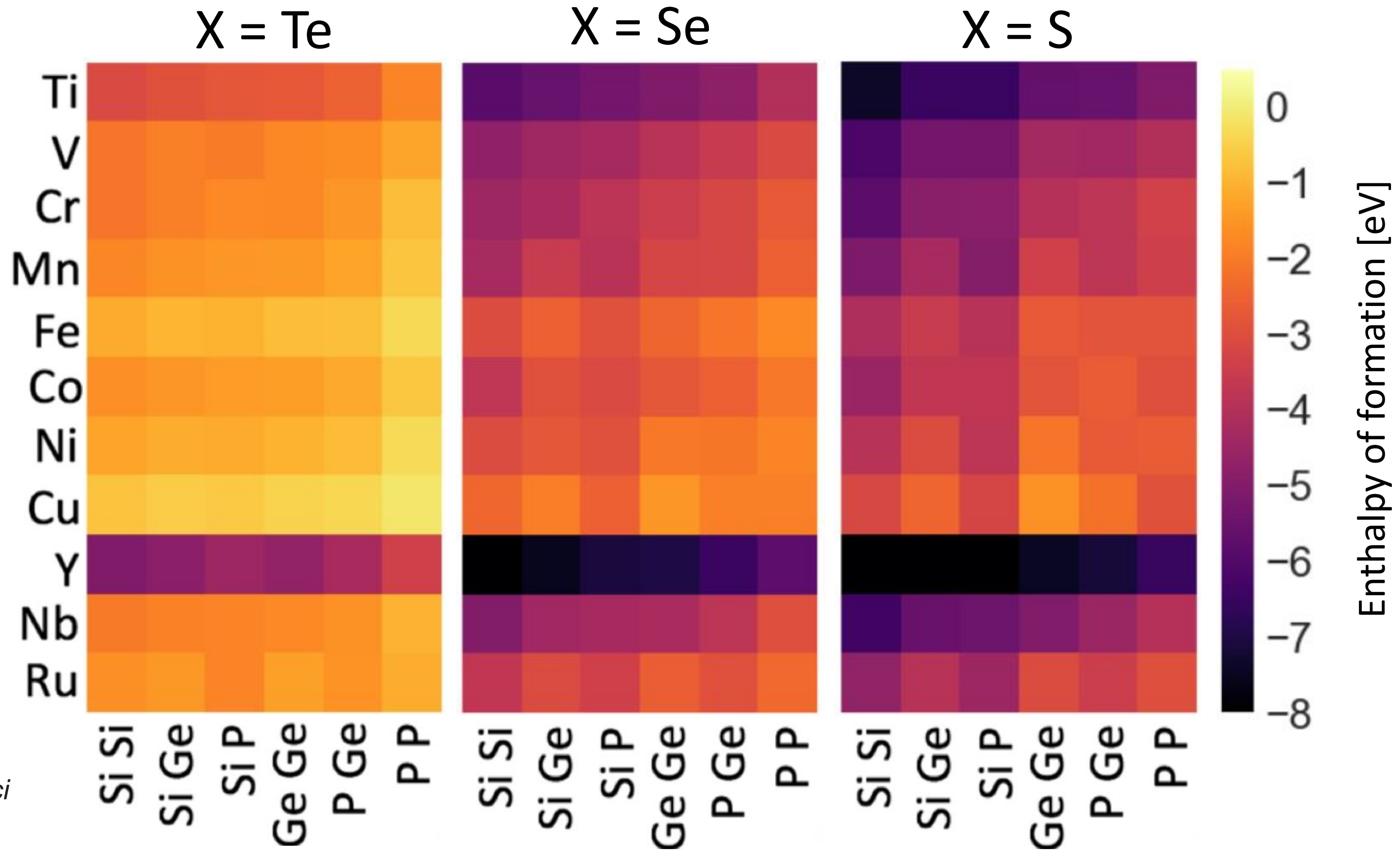
Magnetic moment of $A_2B_2X_6$



Rhone, *et al., Sci Rep* **10,** 15795 (2020).

Formation energy of $A_2B_2X_6$

Formation energy of $A_2B_2X_6$



Rhone, *et al., Sci Rep* **10,** 15795 (2020).

Machine learning in materials science

Materials descriptors

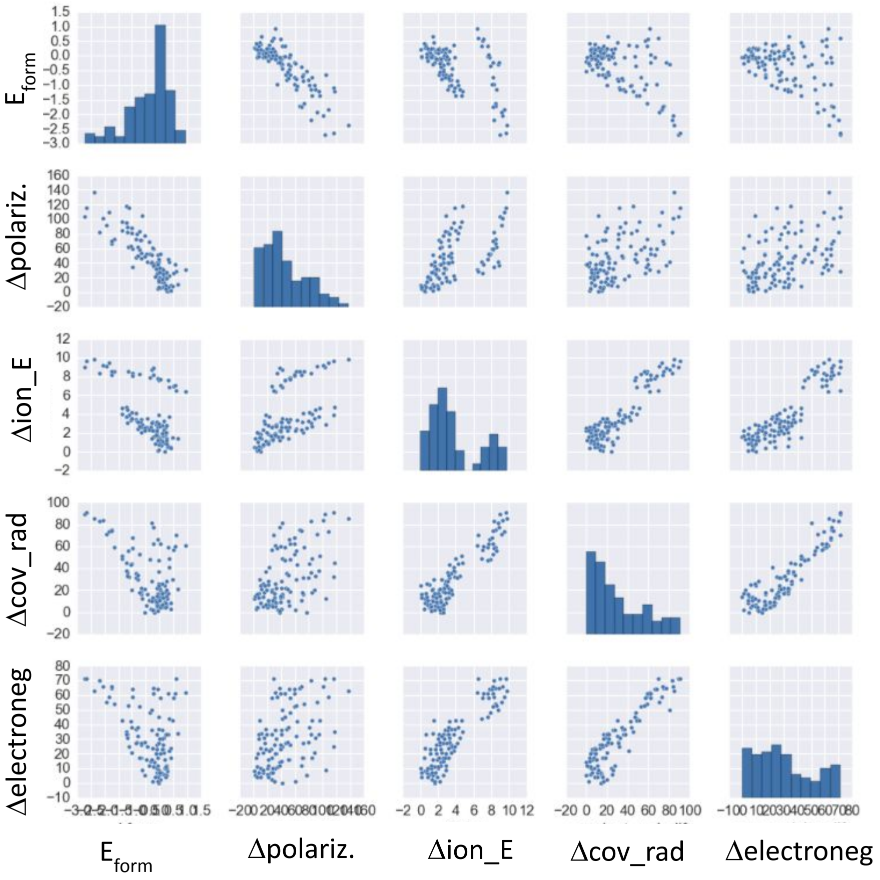
- Describe system using easily attainable components
  - Atomic properties, p
- Compound Property, P
  - mean(p(A), p(B), p(X))
  - variance(p(A), p(B), p(X))
- Total # of descriptors:
  - 61

- Atomic property, p:
  - Number of spin up e's
  - atomic radius
  - etc.

Machine learning in materials science

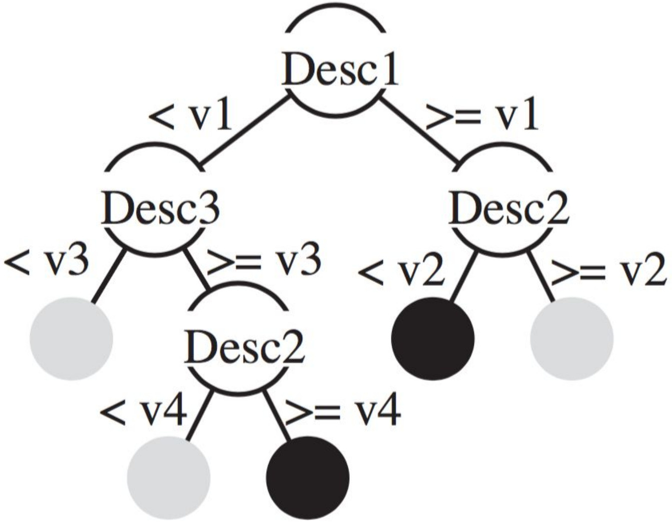
Data visualization

- Atomic properties, p
  - Polarizability
  - Ionization energy
  - Covalent radius
  - electronegativity



Machine Learning models

- Random forest regression
- Inputs: X
  - Number of spin up e's
- Output: Y
  - Magnetic moment
- Training data (70%)
- Test data (30%)



- Node m, region R_m, N_m observations
- Mean Absolute Error
  - minimize L1 error using median values at terminal nodes

$$L(X_m) = \frac{1}{N_m} \sum_{i \in N_m} |y_i - \bar{y_m}|$$

$$\bar{y_m} = \frac{1}{N_m} \sum_{i \in N_m} y_i$$

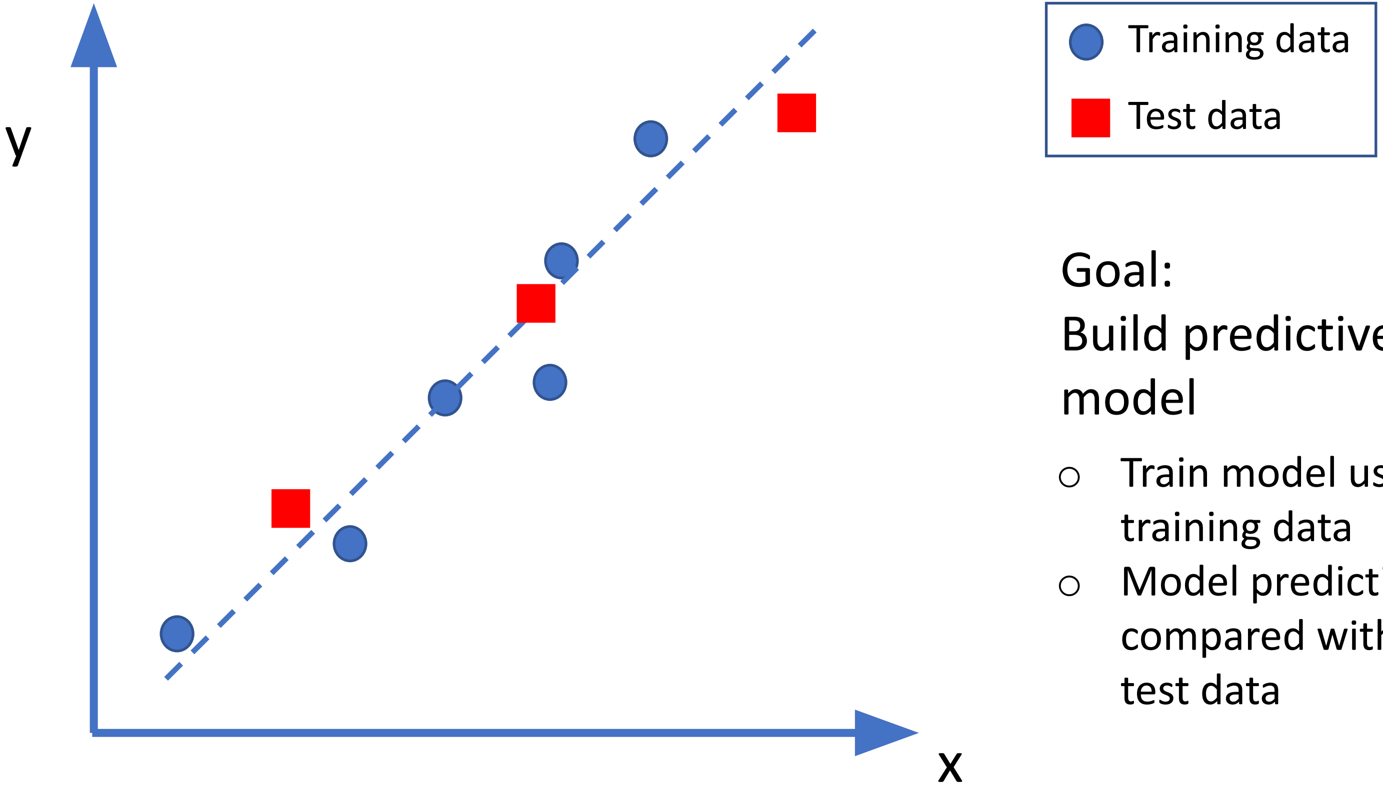
1. G.A. Landrum, H. Genin, Journal of Solid State Chemistry 176 (2003) 587–593

Machine Learning models

Training data versus test data

Machine Learning models

Training data versus test data

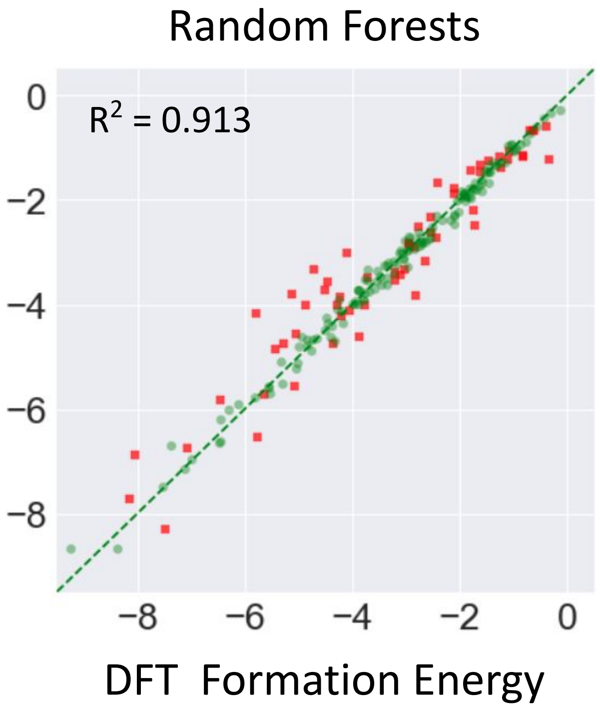


Goal:
Build predictive model

- Train model using training data
- Model predictions compared with test data

Machine learning predictions of DFT formation energy

Machine learning predictions of DFT formation energy



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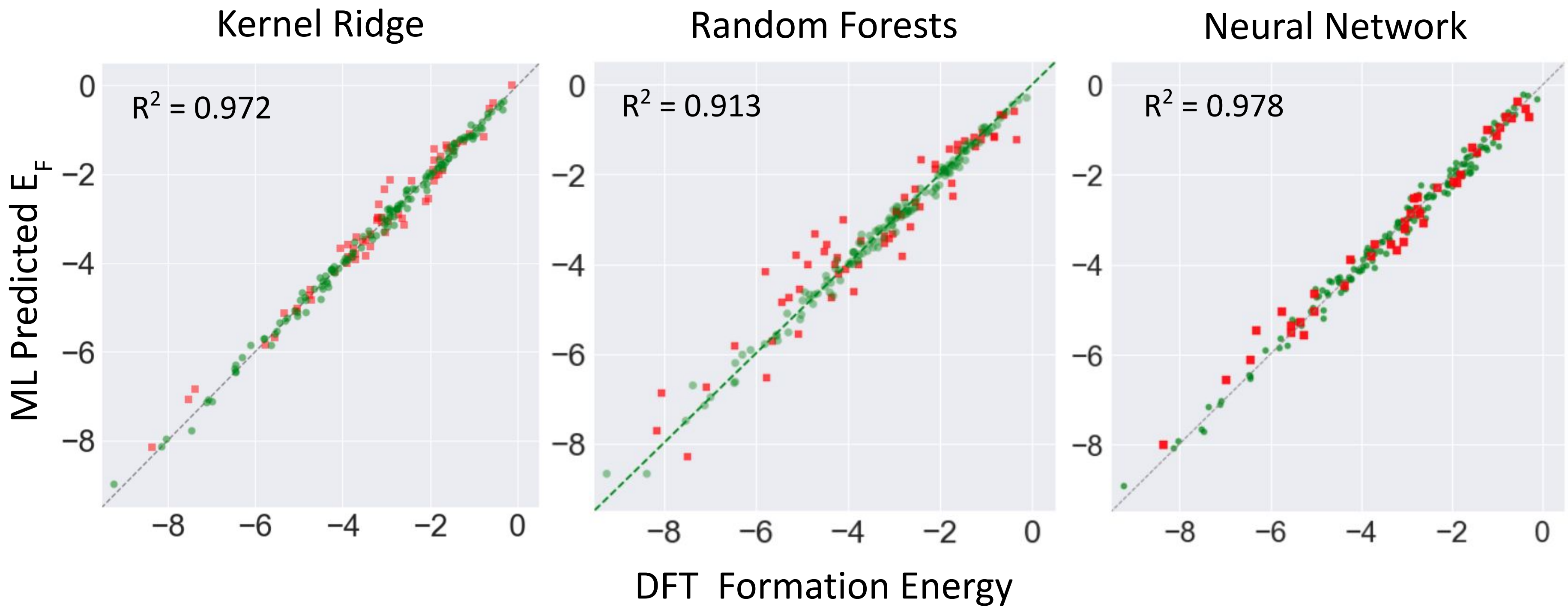
Machine learning predictions of DFT formation energy



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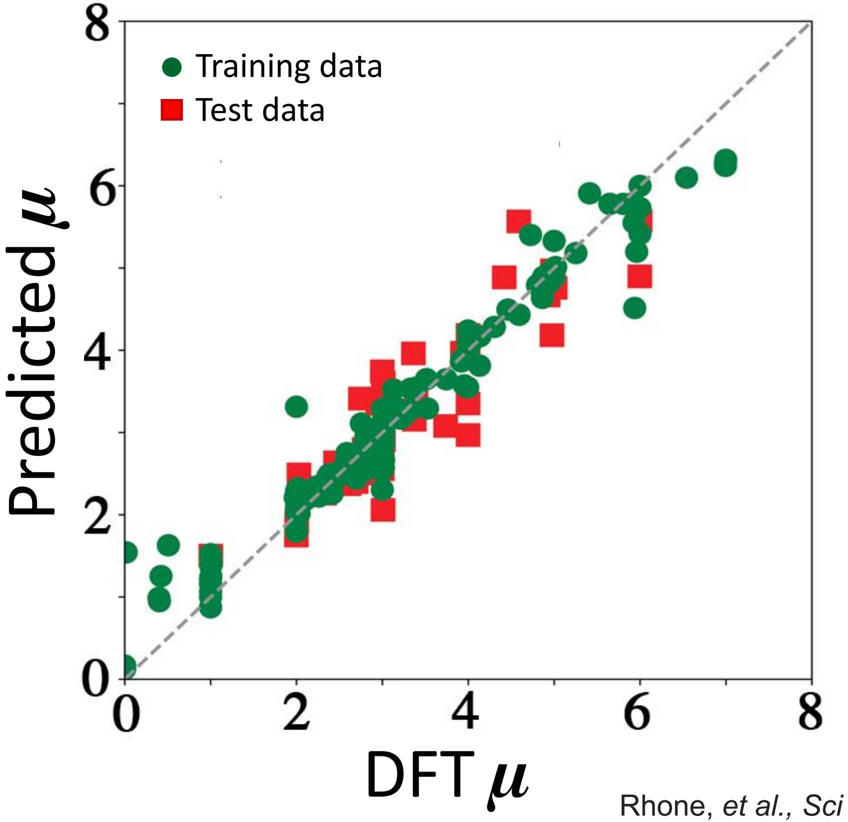
Machine learning predictions
Magnetic moment, X=Te



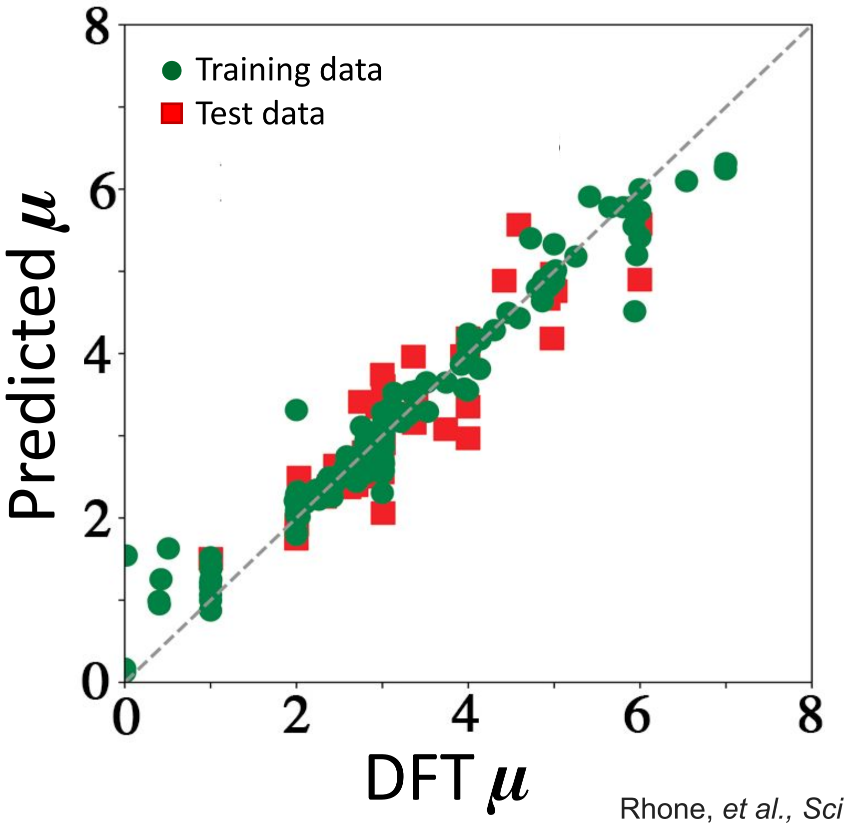
- N = 262
- Random forest R^2 = 0.98
- Mean absolute error (MAE) = 0.30 μ_B

DFT: first-principles quantum calculations

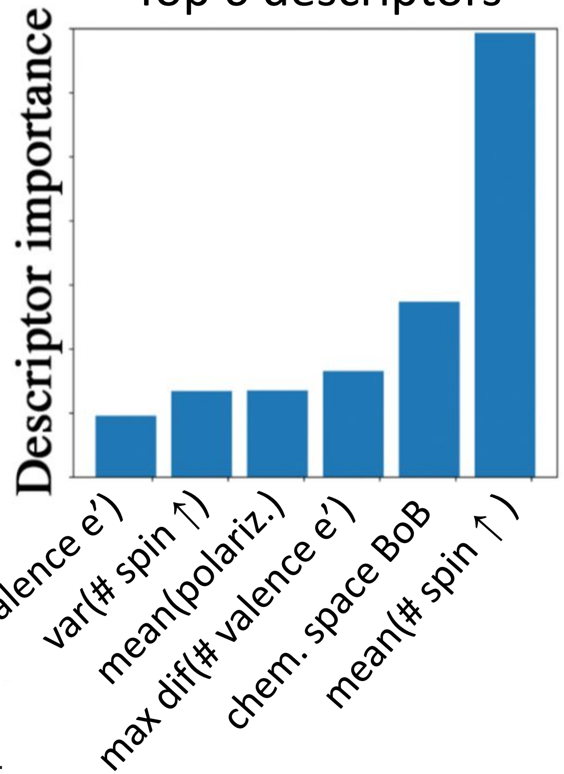
μ: magnetic moment ~ magnetization

Rhone, *et al., Sci Rep* **10,** 15795 (2020).

Machine learning predictions
Magnetic moment, X=Te



Top 6 descriptors



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ML in materials physics education

Overview

1. Physics research: Beginners guide to ML
2. Coursework: ML in physics
3. Workshops: Data science for physicists

ML in physics coursework

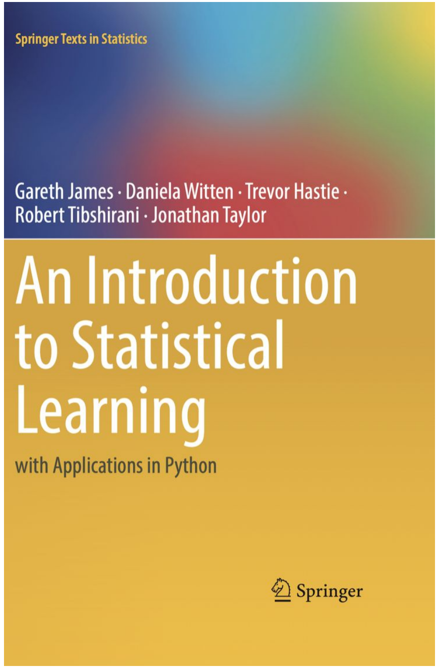
Computational physics course

- 5 lectures on data science:
  - Introduction to data science
  - Introduction to neural networks
  - Neural networks for image analysis

ML in physics coursework

Computational physics course

- Introduction to data science
  - Data mining
  - Data visualization
  - Machine learning models



ML in physics coursework

Computational physics course

- Introduction to data science
  - In-class exercises

scientific reports

Data-driven studies of magnetic two-dimensional materials

Trevor David Rhone, Wei Chen, Shaan Desai, Steven B. Torrisi, Daniel T. Larson, Amir Yacoby & Efthimios Kaxiras

MATERIALSCLOUD

ML in physics coursework

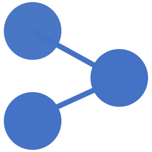
Computational physics course

- Introduction to neural networks
  - Feed forward neural networks
  - Convolutional neural networks

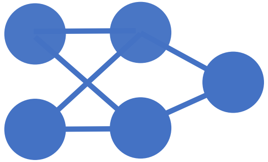
Neural Networks

Architectures

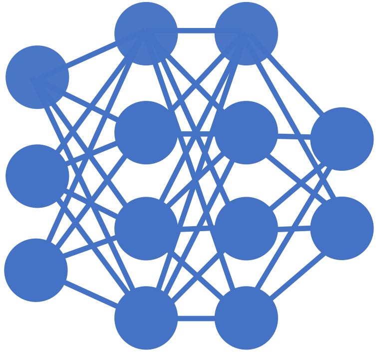
Perceptron



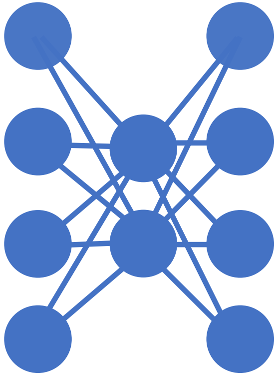
Feed Forward
NN



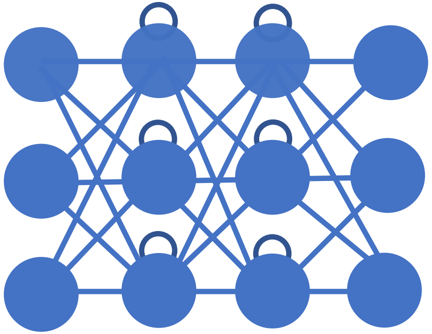
Deep
NN



Autoencoder

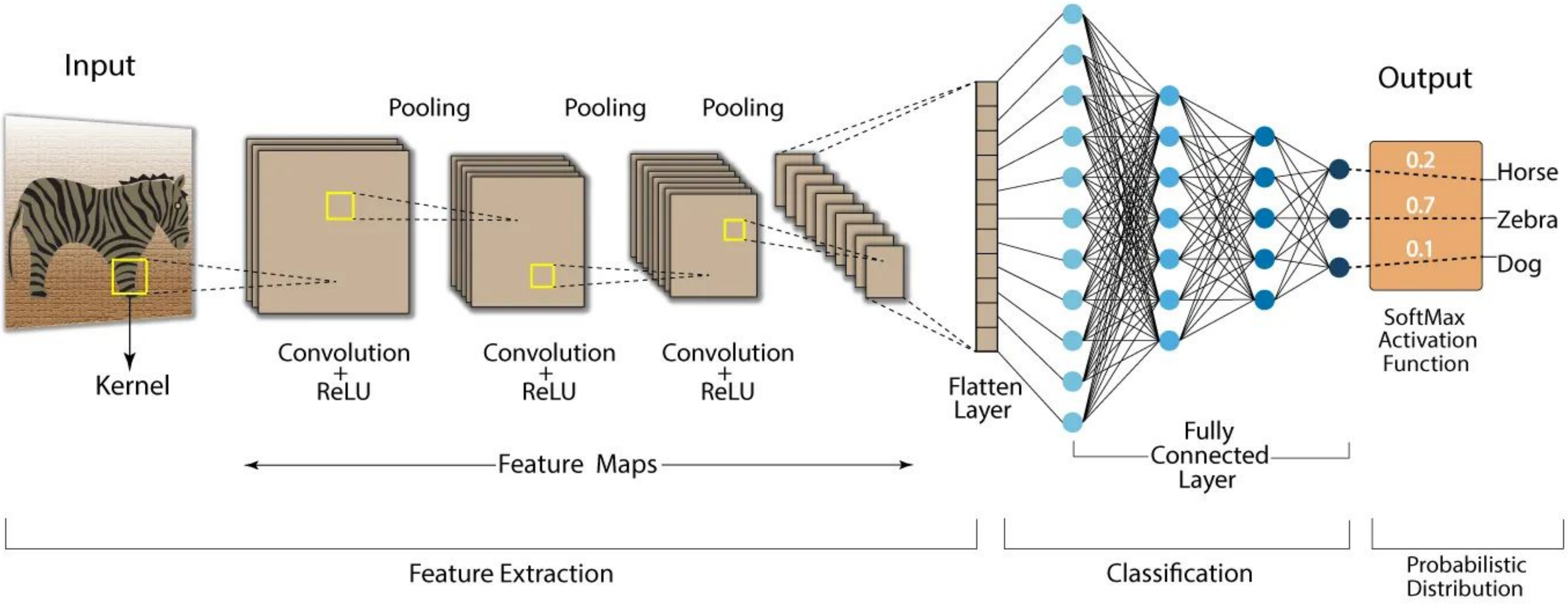


Recurrent
NN



Neural Networks

Convolutional Neural Networks (CNN)



ML in physics coursework

Computational physics course

- Neural networks for image analysis

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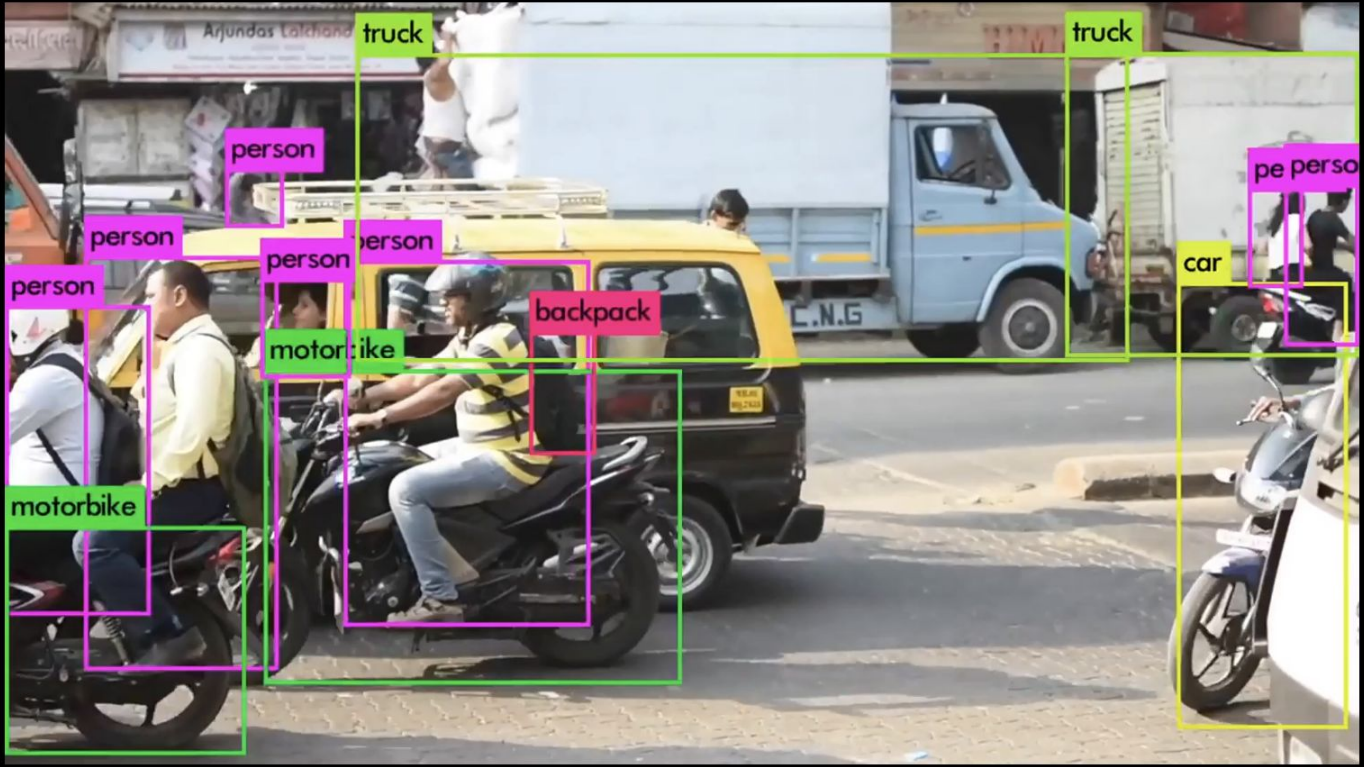
AT HARVARD UNIVERSITY

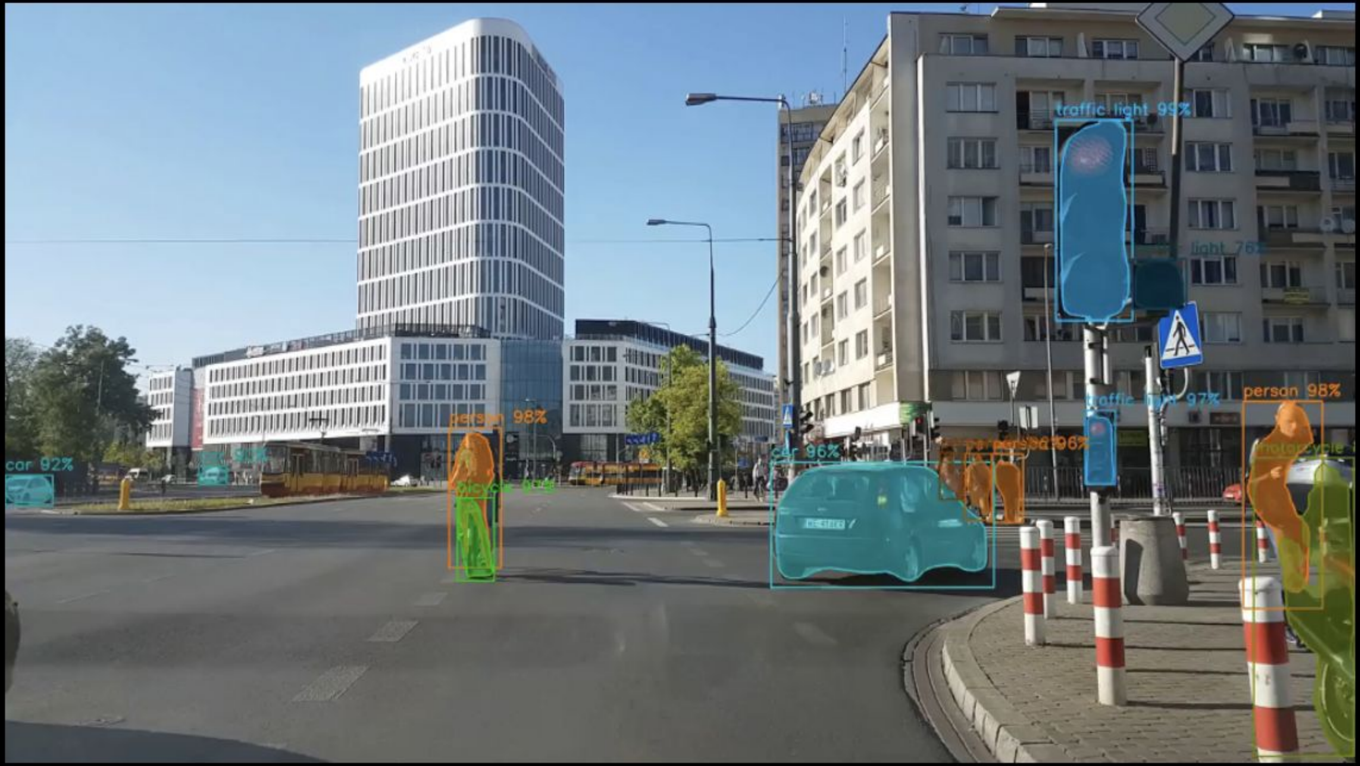
Neural networks for image analysis

You Only Look Once (YOLO) - 2016



Neural networks for image analysis

Mask- RCNN - 2017



ML in physics coursework

Computational physics course

- Neural networks for image analysis

ML in physics coursework

Computational physics course

- Neural networks for image analysis
  - MNIST digits data set
  - Xray images of covid patients

Google colaboratory excercise

COVID-19 RADIOGRAPHY DATABASE

https://www.kaggle.com/datasets/tawsifurrahman/covid19-radiography-database

Database from Kaggle!

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Workshops: Data science for physicists

- **APS Topical Group on Data Science workshop** (2020),
  A beginner's guide to using data science for physicists

- **TWIML AI Symposium** (2020), Webinar,
  Data science education for physicists

- **Magnetic properties from first-principles workshop, Bilkent University** (2021),
  Machine Learning Approaches for Magnetic Characterization

- YouTube tutorials
  - www.materials-intelligence.com

Acknowledgements

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- This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357.

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