WPI

Machine Learning (ML) for MXene Informatics

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CEDAR Grant

National Science Foundation
WHERE DISCOVERIES BEGIN

- Circular Economy and Data Analytics Engineering Research for Sustainability (CEDAR)
- Grant to WPI from the National Science Foundation
  - The project on which I am working is part of the CEDAR grant

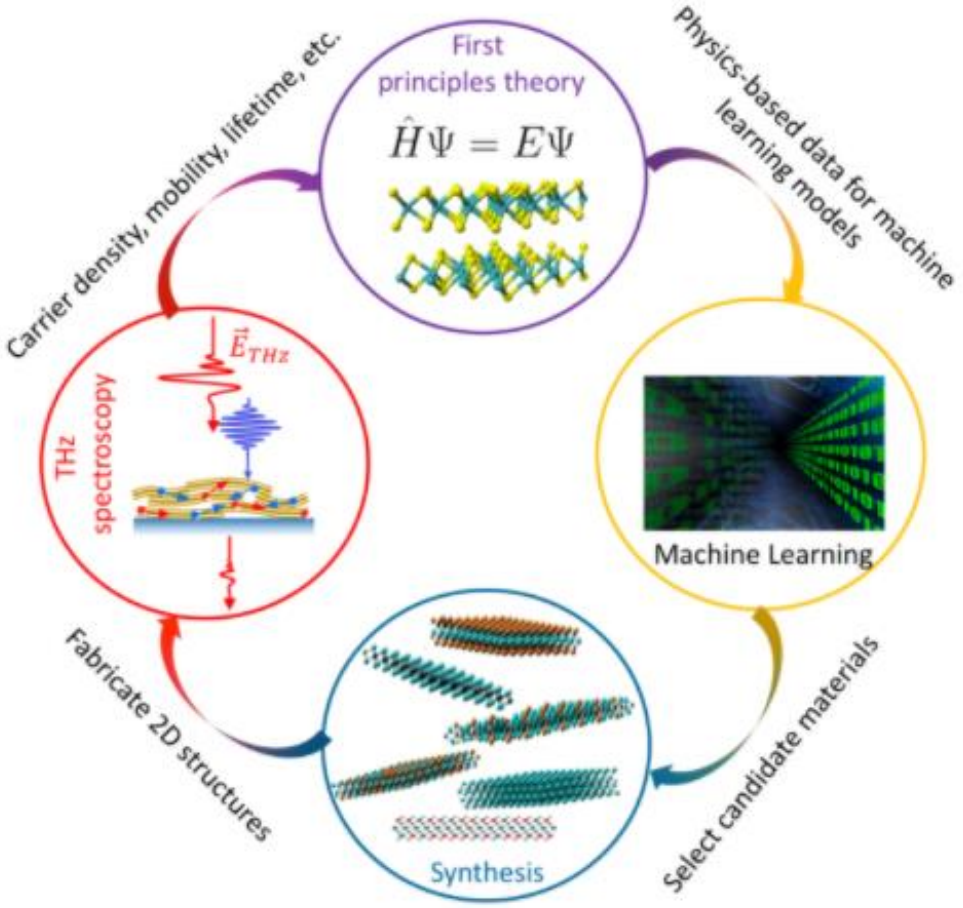
Importance of Predicting Material Properties

- Being able to understand and accurately predict properties of a material would be a gigantic advancement for society
- Information at the atomic level of a material can tell us a ton about properties of that material
  - It turns out that knowing the electronic structure of the atoms in a material can tell us a ton

MXenes Background [1]

- MXenes are a family of 2D materials
- In a 2D flake of MXene, n +1(n = 1−3) layers of early transition metals are interleaved with n layers of carbon or nitrogen, with a general formula of $M_{n+1}X_nT_x$
- The T_x in the formula represents the surface terminations, such as O, OH, F, and/or Cl, which are bonded to the outer M layers

Brief Project overview [2]

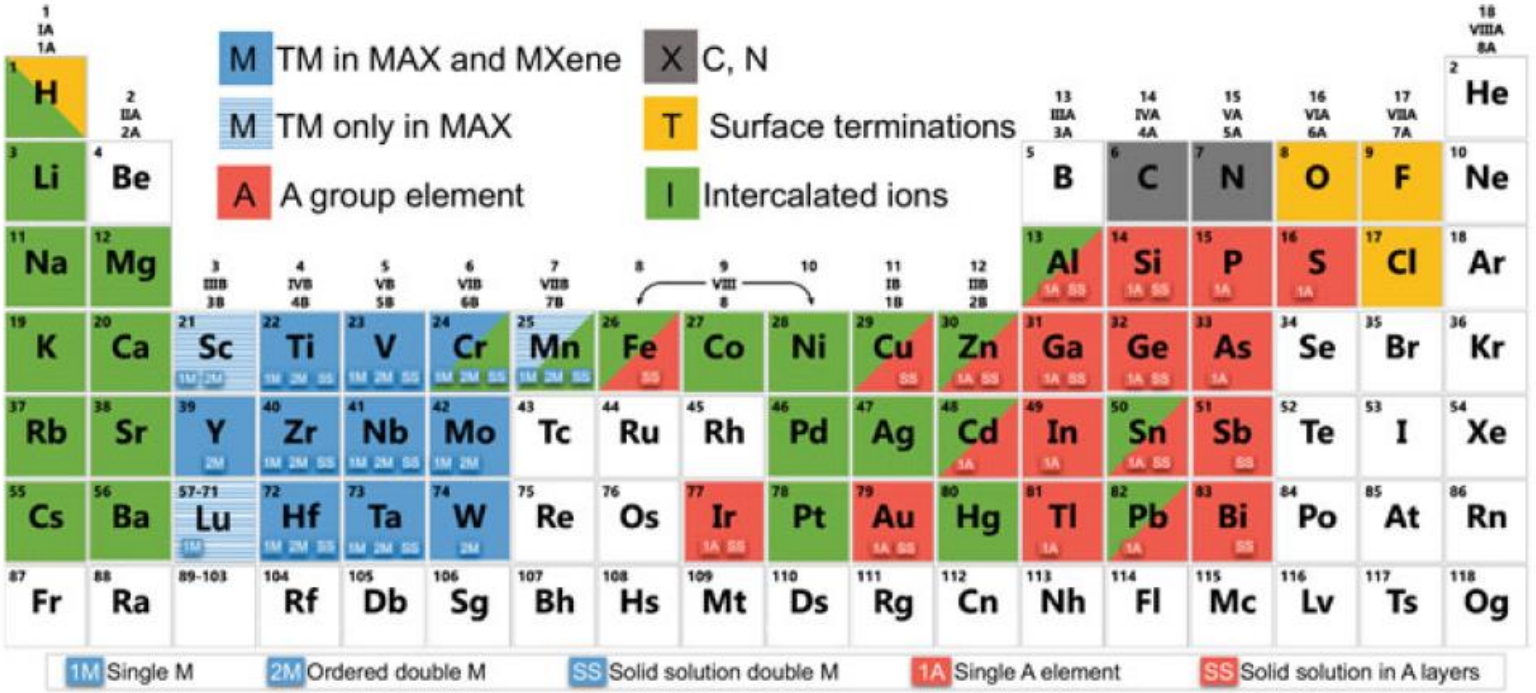


- 4 subgroups
- First Principles & DS teams work together to select MXenes with desired properties
- Drexel lab group synthesize these recommended MXenes
  - Send samples to WPI lab
- WPI Optical Spectroscopy lab analyzes MXene samples to see if they match predictions

UN Sustainable Development Goals (SDGs) [3]

- Predicting MXene properties more accurately, efficiently, and effectively will assist in MXenes being used to their fullest potential
- SDGs this project is associated with:
  - Affordable and Clean Energy
    - MXenes have great potential for improving solar panel efficiency, battery efficiency, supercapacitors, electrodes for Li-S batteries, and transparent conductive electrodes and transparent energy storage devices [1]
  - Industry, Innovation, and Infrastructure
    - In industry, MXenes have many innovative uses
      - E.g. Electromagnetic interference shielding, chemistry and catalysis of MXenes, sensors, and biomedical applications [1]
  - Clean Water and Sanitation
    - MXenes have been used for environmental and water filtration [1]

MXene Constituent Elements [1]



- MXenes, usually created from MAX phases, where "M" elements are in blue, "A" elements in pink (though usually on Al and Si are used), "X" elements in gray, and "T" elements in yellow
  - There are many more "T" elements than listed here

Possible Constituent Elements of MXenes

- List of possible M elements to use:
  - Sc, Ti, V, Cr, Mn, Y, Zr, Nb, Mo, Hf, Ta, W
  - Possibly could use Fe, Co, Ni, Cu, Zn, Tc, Ru, Rh, Pd, Ag, Cd, Re, Os, Ir, Pt, Au, and/or Hg
  - [1] even reported that lanthanides might be able to be MAX phase components
    - Lanthanides go in M layer for MAX phases, but have thus far been unable to synthesize
- List of possible X elements to use:
  - C, N (focus most time on C; N is harder to do)
- List of possible surface terminations to use:
  - Br2, Cl2, CN, F2, H2, H2O2, I2, NCS, NH, NO, O2, OBr, OCl, OCN, OH (might be same as H2O2), PO, PO4, S2, SCN, Se2, Te2, none (aka “bare”),
  - This list can be significantly larger is using additional mixtures

MXene Configurations to try [1,4]

- 2-1, 3-2, 4-3, 5-4, 2-1-2, 1-2-2, 2-2-3, 2-3-4, and 3-2-4
  - An example of 2-1 would be Ti2C, while and example of 2-2-3 would be Cr2V2N2F2
- However, [5] uses four transition metals in the same MXene, for example, TiVNbMoC3Tx (perhaps one could says that this configuration is 1-1-1-1-3)
  - There could also be three transition metals in the same MXene

List of "Desired" Properties of MXenes

- Properties currently working to predict:
  - Fermi Level, Lattice Constant (Å), Band Gap, Work Function, Bader Charge, Elastic Moduli (Young's, shear, bulk), Magnetic (T/F), Metallic (T/F), and Density of States
- Properties that will be attempted to be predicted by the end of summer:
  - Electrical Conductivity, Carrier Density, Carrier Mobility, Carrier Effective Mass, Thermal Conductivity, Seebeck coefficient, Optical Absorption, and Permittivity
- Properties that might be too difficult to predict in the next few months:
  - Carrier Life-time, Sensitivity to Disorder, Reflectivity, Permeability, Charge Recombination, and THz Range (Transmission)

Dataset Description

- Combined two datasets [6, 7] that used Density Functional Theory computational predictions for MXene work functions
  - Training dataset has 275 rows
- Could be up to 14 atoms in a MXene molecule in this dataset
- Replaced each single element with the atomic number of the element

Field Name	**Type**
MXene Name	String
Type of MXene	Categorical
NumberofAtoms	Numeric
M1	Numeric
M2	Numeric
X	Numeric
Surface Termination	Numeric
ChemFormula	Numeric
Period	Numeric
Groupnumber	Numeric

Preliminary Results for Work Function Predictions

- Listed here are the 10 MXenes with the lowest work functions
  - Predicted using Gaussian Process Regression (GPR)
  - MXenes with small work functions have great electronic properties [8]
- Only MXenes with surface terminations of -O, -OH, -F, and bare (no termination) were included here
  - The training data only contains these surface terminations
    - Could possibly cause inaccurate predictions for MXenes with other surface terminations

MXene	Work Function (eV)
Cr5C4H2O2	1.605
Sc5C4H2O2	1.647
Mn5C4H2O2	1.661
Cr2CH2O2	1.706
Y5C4H2O2	1.771
V5C4H2O2	1.796
Mn5N4H2O2	1.826
Mo5C4H2O2	1.829
Ti5C4H2O2	1.890
Cr5N4H2O2	1.906

Long-term Project Goals

- Use ML to find the top-n MXenes based on desired properties
  - e.g. lowest work function
- Then, use DFT on these n MXenes to provide stronger belief (or disbelief) in the ML results
- After this, recommend a new top-k list of MXenes for experimentalists to produce
  - Only include MXenes in the original top-n list where the DFT and ML calculations sufficiently agree are included
- Next, the experimentalists decide which of these top-k MXenes they think are feasible to produce, leaving a final top-q MXenes to attempt to synthesize
- If successful, they will then send the MXene samples to the Optical Spectroscopy Group at WPI
  - Who will then measure the properties of the sample
  - Ideally, they would find MXenes with novel properties that are similar to the predictions!
    - If not, back to the drawing board!

Short-term Project Goals

- Likely not enough time for other parts of the project to finish before end of summer
  - Unlikely that experimentalists will have time to attempt to synthesize these MXenes by end of summer
  - Even less likely that the Spectroscopy Group would be able to analyze MXene samples by end of summer

Issues faced thus far

- Finding data to use to create models to predict these properties has been challenging
  - There is not much experimental data, since producing MXenes is hard!
  - Thus, need to make computational predictions
    - However, it does not appear that there is a large, standardized MXene dataset / database with a large number of properties
    - Even papers that do make computational predictions do not publish their dataset
- It has been difficult to know what input features to use for models
- Predictions thus far do not assess the feasibility of producing these MXenes

Future Work

- The DFT Group is in the process of generating more data
  - This new data will be used to create new models that might perform better than the models outlined in this presentation
  - Will include more surface terminations, increasing the number of permutations of MXenes to examine
- Will create models to predict semiconductor vs. metal
  - Then, after filtering out semiconductors, create models to predict work function
    - Semiconductor work functions are sensitive to the doping level its surface
      - Thus, less useful to predict

Future Work

- Use transfer learning to use data for similar materials for MXene predictions
  - Use storing knowledge gained while solving one problem and applying it to a different but related problem [9]
- Use zero-shot learning to predict properties of MXenes
  - Zero-shot learning is good at providing predictions for training examples that do not have a closely related example in the training data [10]
  - E.g. for MXenes with surface terminations that are not included in the training set, or perhaps MXenes that have more than one transition metal in them
- First-principles group will predict properties of MXenes with 3 or more transition Metals
  - DFT calculations are doable, but need to understand structure to use
    - More atoms requires longer calculations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- [4] Anasori et al. “Two-Dimensional, Ordered, Double Transition Metals Carbides (MXenes).” ACS Nano, 2015.
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- [7] A. C. Rajan, A. Mishra, S. Satsangi, R. Vaish, H. Mizuseki, K. R. Lee and A. K. Singh. Machine-Learning-Assisted Accurate Band Gap Predictions of Functionalized MXene. Chem. Mater., 2018, 30, 4031-4038.
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