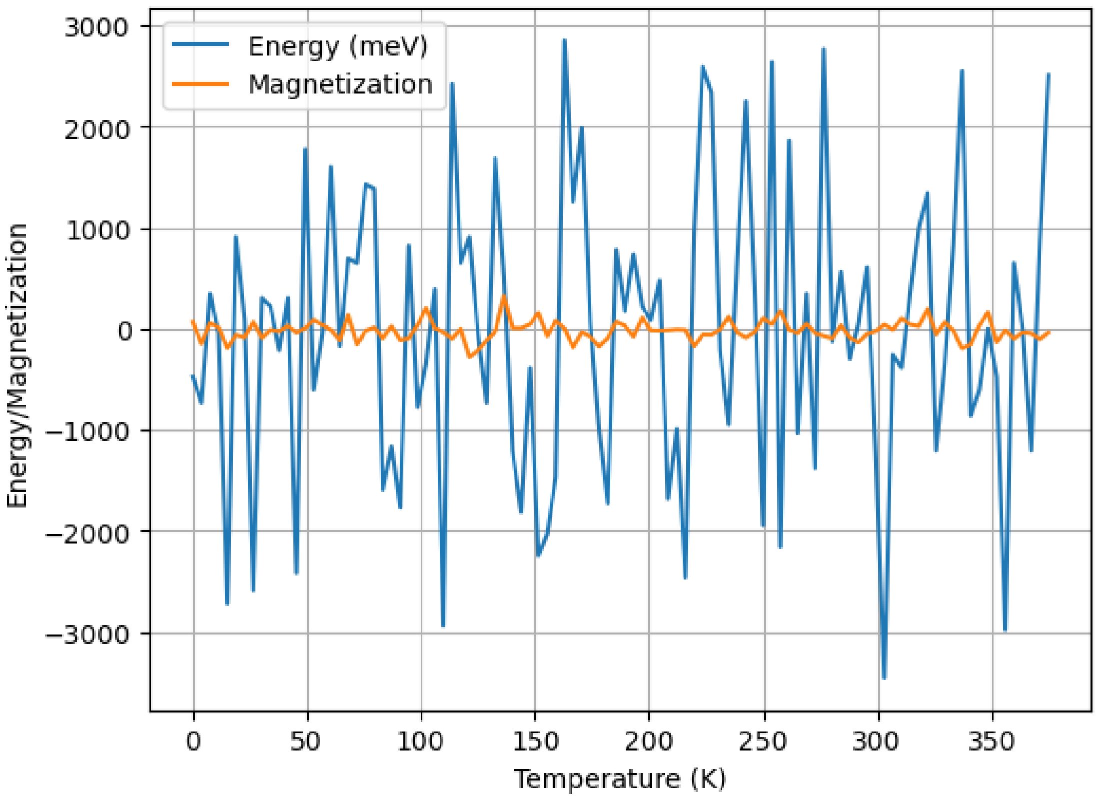
Ising

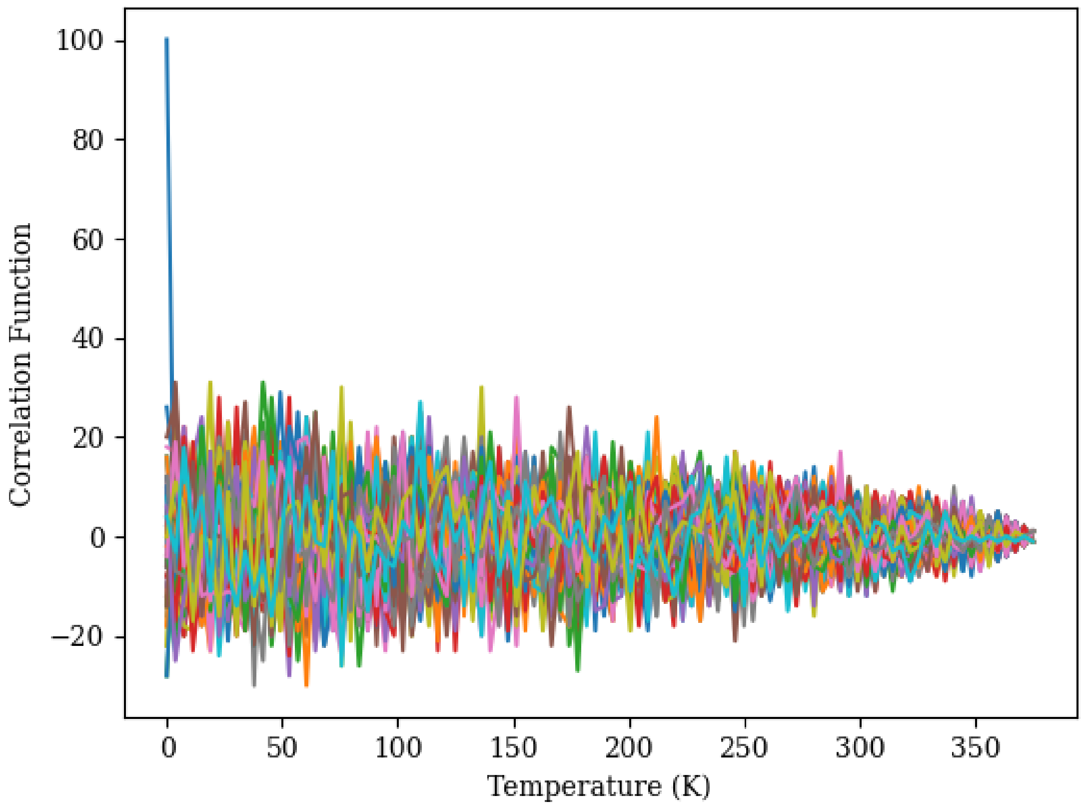
July 6, 2023

[2]:

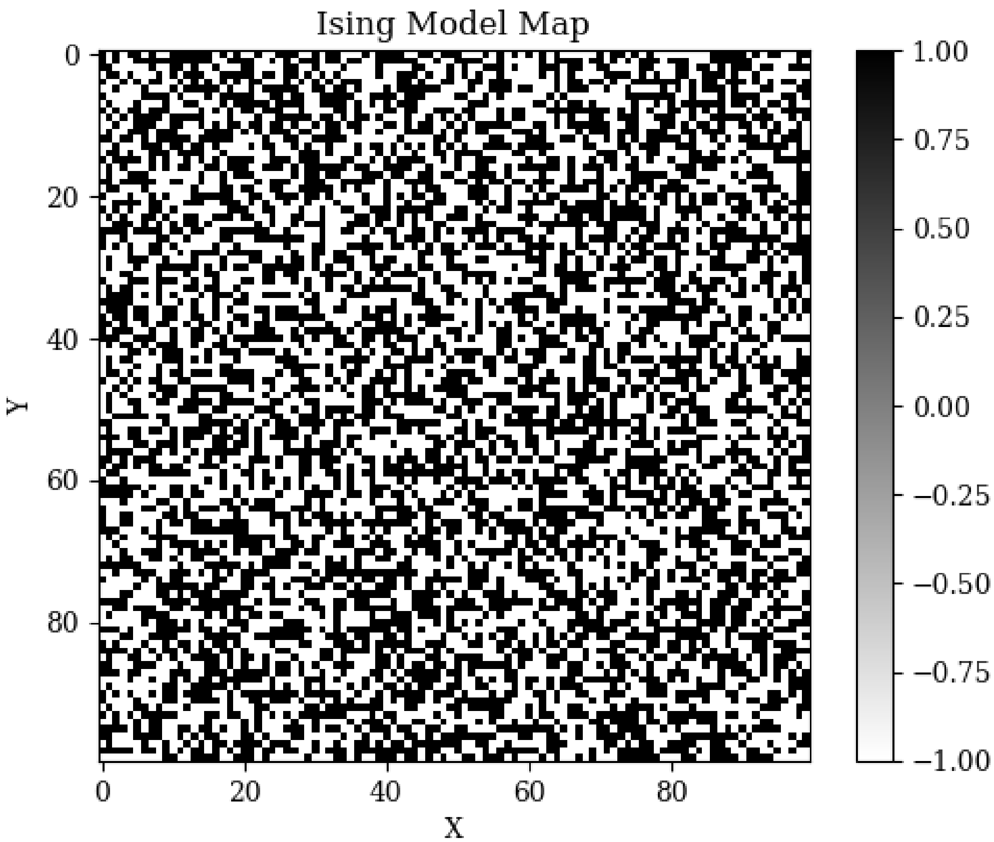
```python
import numpy as np
import matplotlib.pyplot as plt

def ising_model(L, J, T):
  """
  Simulates the Ising model for perovskite materials.

  Args:
    L: System size.
    J: Exchange coupling constant.
    T: Temperature.

  Returns:
    The energy, magnetization, correlation functions, and the Ising model map of␣
↪the system.
  """

  # Initialize the Ising spins.
  spins = np.random.choice([-1, 1], size=(L, L))

  # Calculate the energy of the system.
  energy = -J * np.sum(spins * np.roll(spins, shift=1, axis=0) + spins * np.
↪roll(spins, shift=-1, axis=0) +
                       spins * np.roll(spins, shift=1, axis=1) + spins * np.
↪roll(spins, shift=-1, axis=1))

  # Calculate the magnetization of the system.
  magnetization = np.sum(spins)

  # Calculate the correlation functions.
  correlation_functions = []
  for i in range(L):
    corr = np.correlate(spins[i], spins[0], mode="full")
    corr = corr[L - 1:]
    correlation_functions.append(corr)

  return energy, magnetization, correlation_functions, spins
```

```
if __name__ == "__main__":
  # Set the input parameters.
  L = 100  # System size
  J = 5.4  # Exchange coupling constant
  T_range = np.linspace(0, 375, 100)  # Temperature range

  # Calculate the energy, magnetization, correlation functions, and Ising model␣
↪map of the system for different temperatures.
  energies, magnetizations, correlation_functions, ising_maps = [], [], [], []
  for T in T_range:
    energy, magnetization, correlation_functions, ising_map = ising_model(L, J,␣
↪T)
    energies.append(energy)
    magnetizations.append(magnetization)
    ising_maps.append(ising_map)

  # Plot the energy and magnetization as a function of temperature.
  plt.figure()
  plt.plot(T_range, energies, label="Energy (meV)")
  plt.plot(T_range, magnetizations, label="Magnetization")
  plt.xlabel("Temperature (K)")
  plt.ylabel("Energy/Magnetization")
  plt.legend()
  plt.grid(which="both")
  plt.rcParams['font.family'] = 'serif'
  plt.show()

  # Plot all the correlation functions in the same plot.
  plt.figure()
  for i in range(L):
    plt.plot(T_range, correlation_functions[i], label="Correlation Function")
  plt.xlabel("Temperature (K)")
  plt.ylabel("Correlation Function")
  plt.show()

  # Plot the Ising model map for the final temperature.
  plt.figure()
  plt.imshow(ising_maps[-1], cmap="binary", interpolation="nearest")
  plt.xlabel("X")
  plt.ylabel("Y")
  plt.title("Ising Model Map")
  plt.colorbar()
  plt.show()
```


Energy (meV)
Magnetization
Energy/Magnetization
Temperature (K)
3000
2000
1000
0
−1000
−2000
−3000
0
50
100
150
200
250
300
350



Correlation Function
Temperature (K)
100
80
60
40
20
0
−20
0
50
100
150
200
250
300
350



[3]:
```python
def ising_model(L, J, T, exchange_anisotropy=0, thermal_fluctuations=0):
  """
  Simulates the Ising model for perovskite materials.

  Args:
    L: System size.
    J: Exchange coupling constant.
    T: Temperature.
    exchange_anisotropy: Anisotropy constant.
    thermal_fluctuations: Strength of thermal fluctuations.

  Returns:
    The energy, magnetization, correlation functions, and the Ising model map of␣
↪the system.
  """

  # Initialize the Ising spins.
  spins = np.random.choice([-1, 1], size=(L, L))
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```
    # Calculate the energy of the system.
    energy = -J * np.sum(spins * np.roll(spins, shift=1, axis=0) + spins * np.
 ↪roll(spins, shift=-1, axis=0) +
                        spins * np.roll(spins, shift=1, axis=1) + spins * np.
 ↪roll(spins, shift=-1, axis=1) +
                        2 * exchange_anisotropy * spins * spins)

    # Calculate the magnetization of the system.
    magnetization = np.sum(spins)

    # Calculate the correlation functions.
    correlation_functions = []
    for i in range(L):
      corr = np.correlate(spins[i], spins[0], mode="full")
      corr = corr[L - 1:]
      correlation_functions.append(corr)

    # Apply thermal fluctuations.
    thermal_fluctuations = int(thermal_fluctuations)
    spins += thermal_fluctuations * np.random.randint(-1, 2, size=(L, L))
    spins[spins > 1] = 1
    spins[spins < -1] = -1

    return energy, magnetization, correlation_functions, spins

if __name__ == "__main__":
    # Set the input parameters.
    L = 100  # System size
    J = 5.4  # Exchange coupling constant.
    T_range = np.linspace(0, 375, 100)  # Temperature range
    exchange_anisotropy = 0.1  # Anisotropy constant.
    thermal_fluctuations = 0.1  # Strength of thermal fluctuations.

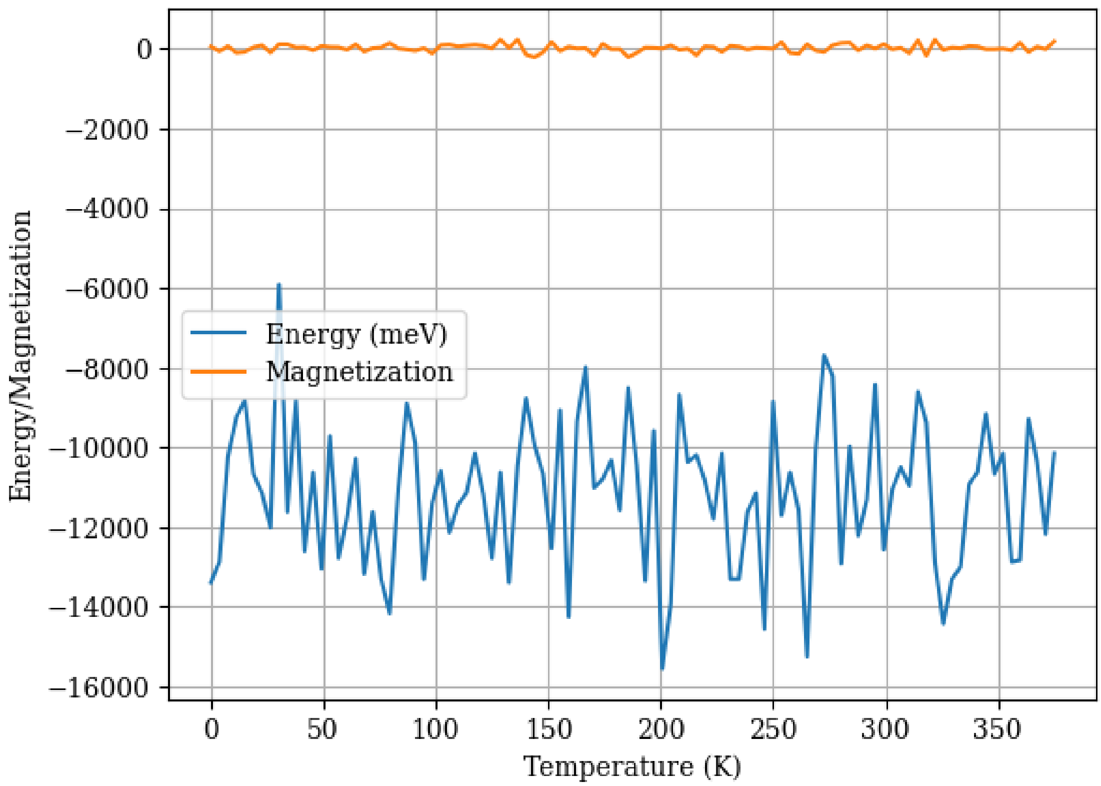
    # Calculate the energy, magnetization, correlation functions, and Ising model␣
 ↪map of the system for different temperatures.
    energies, magnetizations, correlation_functions, ising_maps = [], [], [], []
    for T in T_range:
      energy, magnetization, correlation_functions, ising_map = ising_model(L, J,␣
 ↪T, exchange_anisotropy, thermal_fluctuations)
      energies.append(energy)
      magnetizations.append(magnetization)
      ising_maps.append(ising_map)

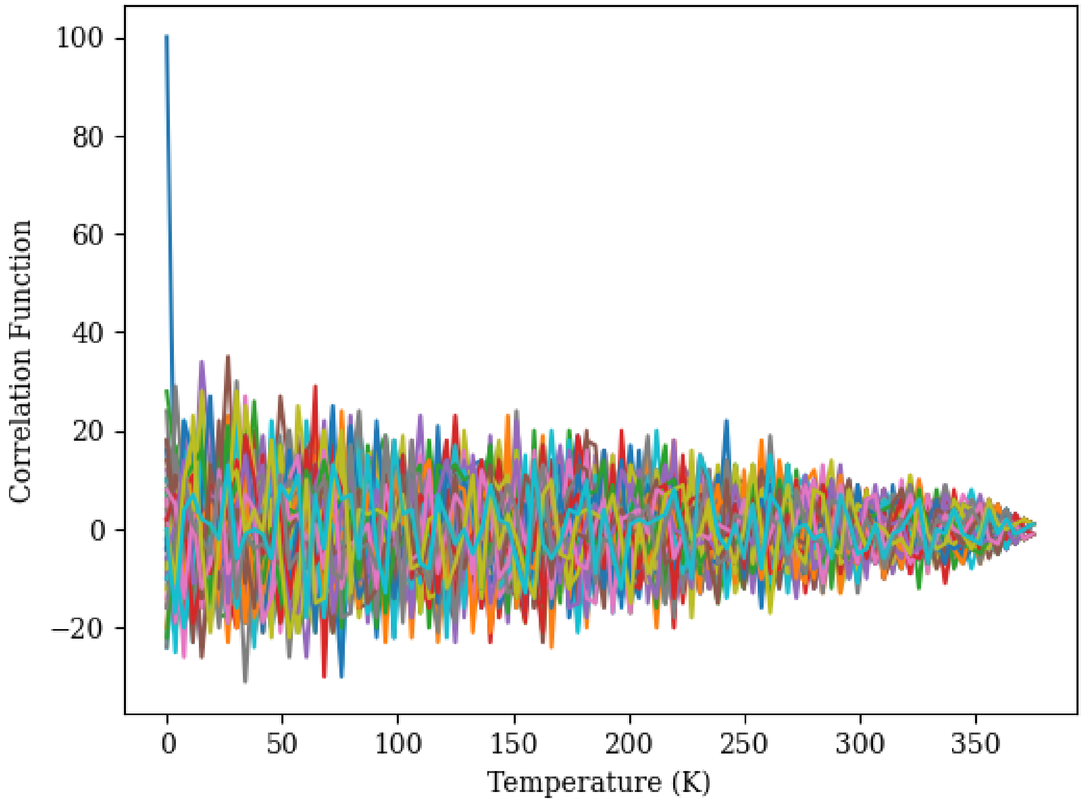
    # Plot the energy and magnetization as a function of temperature.
    plt.figure()
    plt.plot(T_range, energies, label="Energy (meV)")
    plt.plot(T_range, magnetizations, label="Magnetization")
```

```
plt.xlabel("Temperature (K)")
plt.ylabel("Energy/Magnetization")
plt.legend()
plt.grid(which="both")
plt.rcParams['font.family'] = 'serif'
plt.show()

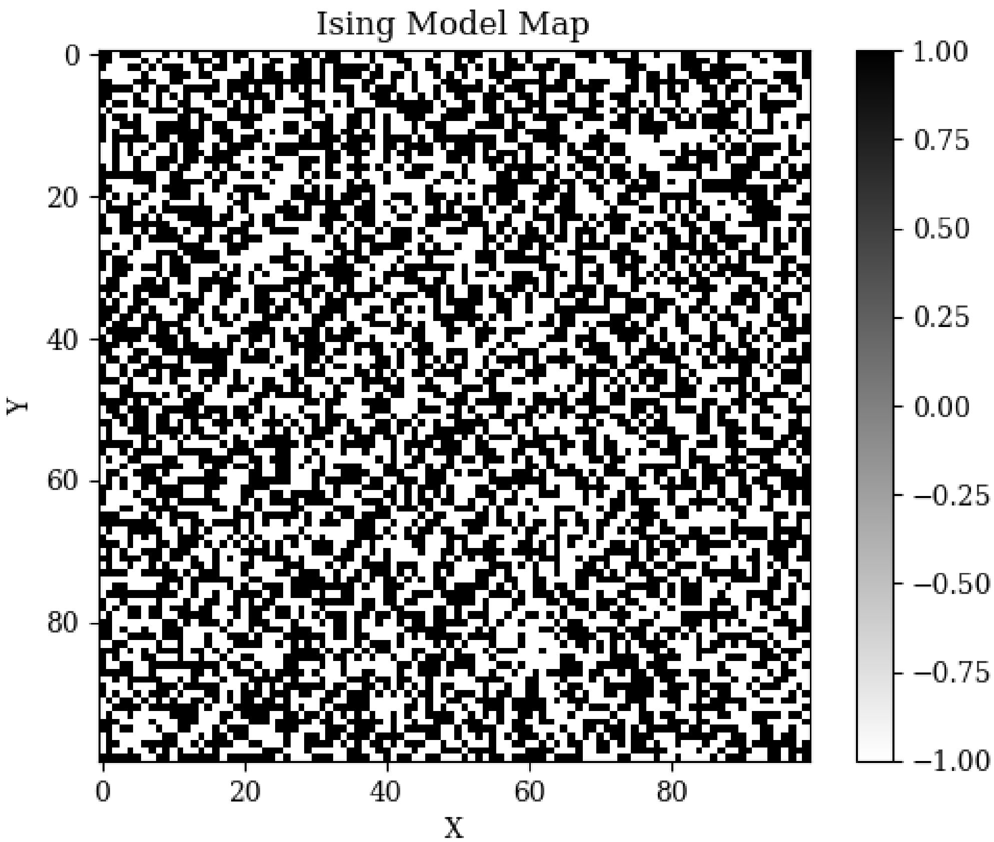
# Plot all the correlation functions in the same plot.
plt.figure()
for i in range(L):
  plt.plot(T_range, correlation_functions[i], label="Correlation Function")
plt.xlabel("Temperature (K)")
plt.ylabel("Correlation Function")
plt.show()

# Plot the Ising model map for the final temperature.
plt.figure()
plt.imshow(ising_maps[-1], cmap="binary", interpolation="nearest")
plt.xlabel("X")
plt.ylabel("Y")
plt.title("Ising Model Map")
plt.colorbar()
plt.show()
```





100
80
60
40
20
0
−20
Correlation Function
0
50
100
150
200
250
300
350
Temperature (K)


Ising Model Map
Y
X
0
20
40
60
80
0
20
40
60
80
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00

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[ ]:
```