Fermi Energy Plot for Na at Different Temperatures

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1 Introduction

This document describes the computational process and mathematical expressions used to generate a Fermi energy plot for sodium (Na) at different temperatures.

2 Mathematical Expressions

The Fermi-Dirac distribution function is given by:

$$f(E,T) = \frac{1}{1 + e^{\frac{E-E_f}{k_B T}}} \tag{1}$$

where:

$$\begin{aligned} E &: \text{Energy (eV)} \\ E_f &: \text{ Fermi energy (eV)} \\ k_B &: \text{Boltzmann constant } (8.617333262145 \times 10^{-5}\,\text{eV/K}) \\ T &: \text{Temperature (K)} \end{aligned}$$

At zero temperature ($T = 0\,\text{K}$), the Fermi-Dirac distribution behaves as a step function:

$$f(E,0) = \frac{1}{2}\left(1 + \text{sign}(E_f - E)\right) \tag{2}$$

- When $E > E_f$, the argument of the sign function becomes positive, and $\text{sign}(E_f - E)$ evaluates to $+1$. The step function then becomes $\frac{1}{2}(1+1) = 1$, indicating that states with energy E above the Fermi energy E_f are fully occupied at absolute zero.
- At exactly $E = E_f$, the argument of the sign function becomes zero, and $\text{sign}(0) = 0$. The step function evaluates to $\frac{1}{2}(1 + 0) = \frac{1}{2}$, signifying that states with energy exactly equal to the Fermi energy have a probability of being occupied equal to $\frac{1}{2}$ at absolute zero.

3 Computational Process

The computational process involves the following steps:

1. Define constants such as the Boltzmann constant k_B and the given Fermi energy E_f.
2. Specify a range of temperatures and an energy range for the plot.
3. Calculate the Fermi-Dirac distribution for each temperature using the defined mathematical expressions.
4. Plot the results using the Matplotlib library in Python.

4 Results

The generated plot illustrates the Fermi energy at different temperatures for sodium.