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# -*- coding: utf-8 -*-

"""
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ME 5110: Advanced Thermodynamics
Homework 04
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"""

import matplotlib.pyplot as plt
import numpy as np

# -----
#PROBLEM 03b
# -----


#Define Variables
De = 7.31*10**-19 #Units: J
a = 1.81*10**10 #Units: 1/m
Re = 1.275*10**-10 #Equilibrium bond length (Units: m)
k = 2*De*a**2 #Force constant (Units: N/m)

#Generate Actual Bond Lengths
R = np.linspace(0.5*Re, 1.5*Re, 10000) #Units: m
x = R - Re

#Define Morse Potential
U_morse = De*(np.exp(-2*a*x) - 2*np.exp(-a*x) +1) #Units: J

#Define Corresponding Harmonic Oscillator Potential
U_harmonic = 0.5*k*x**2 #Units: J

#Conversions
R_pm = R * 10**12 #Actual Bond Lengths (Units: pm)

#Create Plot
plt.figure("Morse Potential vs Harmonic Oscillator Potential for HCl", figsize=(8,5))
plt.plot(R_pm, U_morse, label='Morse Potential', color ='blue')
plt.plot(R_pm, U_harmonic, linestyle=':', label='Harmonic Oscillator Potential', color='Red')
plt.xlabel('Bond Length, R (pm)')
plt.ylabel('Potential Energy, U (J)')
plt.title('Morse Potential vs Harmonic Oscillator Potential for HCl')
plt.legend(loc='upper right', bbox_to_anchor=(1, 0.5))
plt.tight_layout()
plt.show()

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