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In [19]: import pandas as pd
import matplotlib.pyplot as plt
import numpy as np

# -----
# 1. Create Beer's Law dataset
# -----
data = {
    "Concentration": [0.00000, 0.00050, 0.00100, 0.00150, 0.00200, 0.00250, 0.00300,
    "Absorbance": [0.012, 0.091, 0.162, 0.238, 0.313, 0.381, 0.460,
}

df = pd.DataFrame(data)

# -----
# 2. Plot raw calibration data
# -----
plt.scatter(df["Concentration"], df["Absorbance"])
plt.xlabel("Concentration (M)")
plt.ylabel("Absorbance")
plt.title("Beer's Law Calibration Data")
plt.grid(True)
plt.show()

# -----
# 3. Linear regression ( $A = mC + b$ )
# -----
x = df["Concentration"].values
y = df["Absorbance"].values

# Fit best-fit line
m, b = np.polyfit(x, y, 1)

print("Slope (m):", m)
print("Intercept (b):", b)

# Predicted absorbances
y_pred = m * x + b

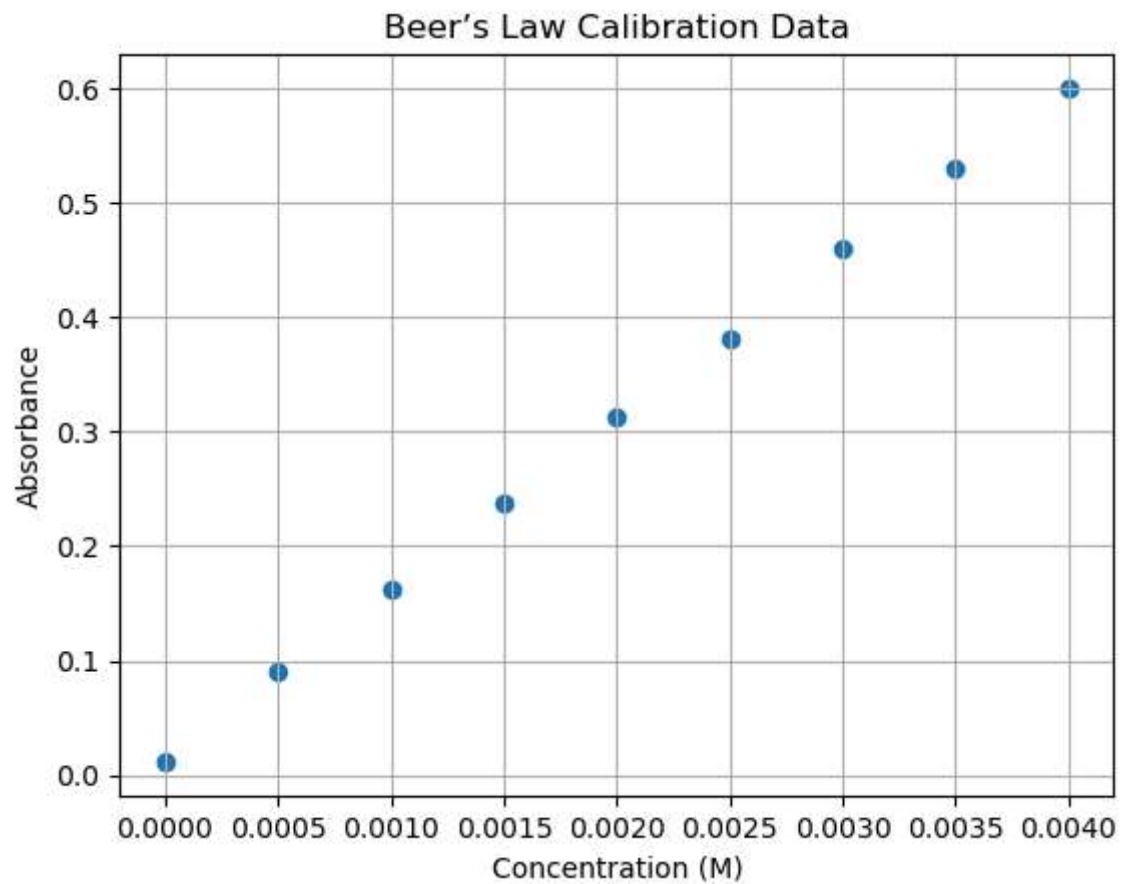
# R-squared (goodness of fit)
ss_res = np.sum((y - y_pred)**2)
ss_tot = np.sum((y - np.mean(y))**2)
r_squared = 1 - (ss_res / ss_tot)

print("R^2:", r_squared)

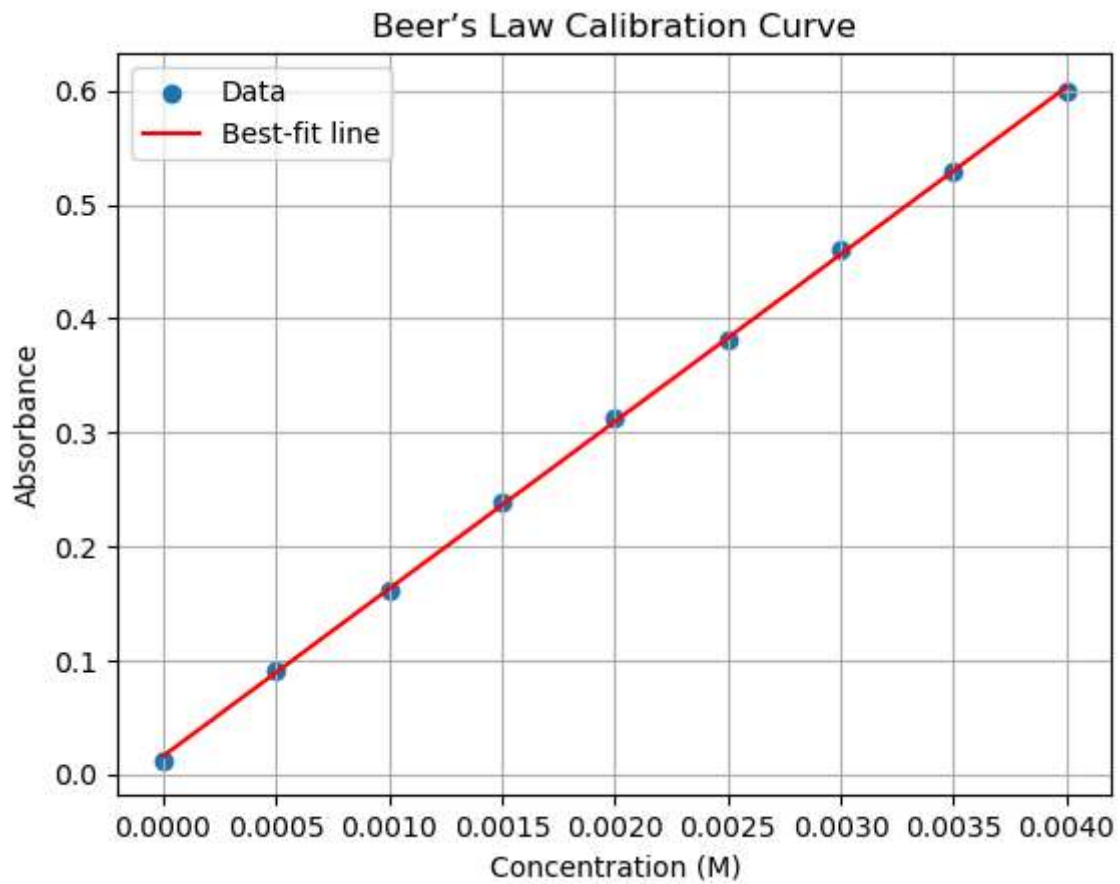
# -----
# 4. Plot best-fit line
# -----
plt.scatter(x, y, label="Data")
plt.plot(x, y_pred, color="red", label="Best-fit line")
plt.xlabel("Concentration (M)")
plt.ylabel("Absorbance")
plt.title("Beer's Law Calibration Curve")

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plt.grid(True)  
plt.legend()  
plt.show()
```



Slope (m): 146.83333333333333
Intercept (b): 0.015888888888888876
 R^2 : 0.9998089249646189



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In [20]: plt.savefig("beers_law_calibration_curve.png", dpi=300)
plt.show()
```

<Figure size 640x480 with 0 Axes>

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In [ ]:
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