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Numerical Optimization

In this lecture we will continue to work with the ethanol peaks dataset and look at numerical optimization from the perspective of non-linear regression.

First, we can re-load the dataset and select the same region we were working on before:

In [1]:
```
%matplotlib inline
import pandas as pd
from matplotlib import pyplot as plt
plt.style.use('../settings/plot_style.mplstyle')

df = pd.read_csv('data/ethanol_IR.csv')
x_all = df['wavenumber [cm^-1]'].values
y_all = df['absorbance'].values

x_peak = x_all[475:575]
y_peak = y_all[475:575]

fig, ax = plt.subplots()
ax.plot(x_peak,y_peak, '-', marker='.')
ax.set_xlabel('wavenumber [cm^-1]')
ax.set_ylabel('absorbance');
```