Auswertung mit Python

February 1, 2026

1 Auswertung 27.05.2025

Auswertung mit vergleich von TBBB TCBC und LNO

1.1 Präambel

[100]:
```python
import numpy as np
import matplotlib.pyplot as plt
from matplotlib import cm
from scipy.optimize import curve_fit

import glob
import re

def dat2array(file_path):
    data = []
    with open(file_path, 'r', encoding='utf-8') as file:
        for i, line in enumerate(file):
            line = line.replace(',', '.').replace('\t', ';').replace('\n', '')
            if i >= 39:  # Skip header lines
                data.append(line.split(';'))

    freqs = [float(row[0]) for row in data]
    intensities = [float(row[1]) for row in data]
    return freqs, intensities

def extract_info(filename):
    match = re.search(r'0(\d+)_(\d+)K\.asc', filename)
    if match:
        return int(match.group(1)), int(match.group(2))
    return None, None

def gaussian(x, a, mean, sigma):
    return a * np.exp(-(x - mean) ** 2 / (2 * sigma ** 2))
```

[101]:
```python
 # Hilfsfunktion: FWHM aus diskreten Daten via linearer Interpolation bestimmen
def _compute_fwhm_from_discrete(x, y, ymax=None):
    if x is None or y is None or len(x) == 0 or len(y) == 0:
```

```python
        return None
    if ymax is None:
        ymax = max(y)
    half = ymax / 2.0
    idx_max = int(np.argmax(y))
    # Linke Halbwertsstelle
    left = None
    for i in range(idx_max, 0, -1):
        y1, y2 = y[i-1], y[i]
        if (y1 - half) * (y2 - half) <= 0:  # Vorzeichenwechsel bzw. Schnitt
            x1, x2 = x[i-1], x[i]
            if y2 != y1:
                left = x1 + (half - y1) * (x2 - x1) / (y2 - y1)
            else:
                left = x[i]
            break
    # Rechte Halbwertsstelle
    right = None
    for i in range(idx_max, len(y) - 1):
        y1, y2 = y[i], y[i+1]
        if (y1 - half) * (y2 - half) <= 0:
            x1, x2 = x[i], x[i+1]
            if y2 != y1:
                right = x1 + (half - y1) * (x2 - x1) / (y2 - y1)
            else:
                right = x[i]
            break
    if left is None or right is None:
        return None
    return abs(right - left)
```

[102]:

```python
def NLO_plot(middle_value, difference, filepath, suptitle, filename_prefix,␣
 ↪reference=False, compare=True, power="333µW", slit_width="210µm",␣
 ↪plotting="energy", normalisationfactor=3.7490887328811729e+12,␣
 ↪norm_intensitaet=6.6181976473128055e+13, refmeas="LNO-SHG"):
    # Suffix für Dateiname wenn wavelength gepottet wird
    if plotting.lower() != "energy":
        filename_prefix += "_wavelength"

    # x_range: Filterung immer noch in nm (basiert auf Input-Parametern)
    x_range = (middle_value - difference, middle_value + difference)
    file_list = glob.glob(filepath)

    sorted_files = []
    for f in file_list:
        meas_no, temperature = extract_info(f)
        if meas_no is not None:
```

```python
            sorted_files.append((f, meas_no, temperature))

    sorted_files.sort(key=lambda x: x[1])

    # Automatische Erkennung des Umkehrpunkts (Peak-Temperatur)
    if sorted_files:
        temps = [x[2] for x in sorted_files]
        max_idx = temps.index(max(temps))
    else:
        max_idx = -1

    extended_files = []
    for i, (f, meas_no, temperature) in enumerate(sorted_files):
        # Bis zum Maximum (inklusive) ist heating=True, danach False
        heating = (i <= max_idx)
        extended_files.append((f, meas_no, temperature, heating))

    temperatures = [x[2] for x in sorted_files]
    if len(temperatures) == 0:
        print("Keine Dateien gefunden, die dem Pfad entsprechen.")
        return
    norm = plt.Normalize(min(temperatures), max(temperatures))
    colors = cm.plasma(norm(temperatures))

    fig, (ax0, ax1) = plt.subplots(1, 2, figsize=(15, 5))
    peak_list = []
    temps_for_line = []
    peaks_for_line = []

    # Sammle Peak-Parameter je Messung für spätere Zusammenfassung
    peak_metrics = [] # Einträge: dict(...)

    for idx, (f, meas_no, temperature, heating) in enumerate(extended_files):
        freqs, intensities = dat2array(f) # nm, arb. u.

        # 1. Referenzkorrektur der Intensität (falls nötig, z.B. ND Filter, Zeit)
        if reference:
            intensities = [val * 32.88 * (10/7) for val in intensities]

        # 2. Daten filtern (im Wellenlängenbereich)
        # Wir filtern zuerst in nm, da middle_value/difference in nm sind.
        filtered_data = [(fr, i) for fr, i in zip(freqs, intensities) if x_range[0] <= fr <= x_range[1]]

        if not filtered_data:
            continue
```

```
        freqs_vec, ints_vec = zip(*filtered_data)
        freqs_vec = np.array(freqs_vec)
        ints_vec = np.array(ints_vec)

        # 3. Transformation (Wellenlänge vs. Energie)
        if plotting.lower() == "energy":
            # Umrechnung nm -> eV
            # E = hc / lambda. hc approx 1239.84 eV nm
            x_vals = 1239.84 / freqs_vec

            # Jacobian Transformation für Intensität: I(E) = I(lambda) *␣
↪lambda^2 / hc
            # Konstante hc ignorieren wir bei arb. u. -> I(E) ~ I(lambda) *␣
↪lambda^2
            # Intensität skaliert mit Quadrat der Wellenlänge
            y_vals = ints_vec * (freqs_vec ** 2)

            # Sortieren, da 1/x die Reihenfolge umkehrt
            sort_idx = np.argsort(x_vals)
            x_vals = x_vals[sort_idx]
            y_vals = y_vals[sort_idx]

        else:
            # Wavelength plotting
            x_vals = freqs_vec
            y_vals = ints_vec

        # 4. Normierung für den linken Plot (Intensität)
        # Wenn norm_intensitaet=1, wird nichts geändert.
        y_vals_plot = y_vals / norm_intensitaet

        # Plotten der Messdaten
        ax0.plot(x_vals, y_vals_plot, color='lightgray', alpha=0.5, linewidth=0.
↪5)

        # --- Temperaturwert für rechten Plot ---
        temp_for_plot = temperature

        # 5. Gaussian Fit & Fläche
        try:
            # Startwerte schätzen
            # Amplitude, Mean, Sigma
            p0 = [np.max(y_vals), np.mean(x_vals), (np.max(x_vals)-np.
↪min(x_vals))/10]

            popt, _ = curve_fit(gaussian, x_vals, y_vals, p0=p0, maxfev=5000)
```

```
            fitted_curve = gaussian(x_vals, *popt)

            # Plot Fit (normiert auf Höhe im linken Plot)
            ax0.plot(x_vals, fitted_curve / norm_intensitaet, color=colors[idx])

            # Fläche unter der Kurve (Trapez) oder Integral des Fits
            area = np.trapezoid(fitted_curve, x_vals)
            if area < 0: area = abs(area)

            # Peak-Parameter
            a_fit = popt[0]
            mean_fit = popt[1]
            sigma_fit = abs(popt[2])
            fwhm_fit = 2.0 * np.sqrt(2.0 * np.log(2.0)) * sigma_fit # ~2.355 *
↪sigma

            peak_metrics.append({
                'height': a_fit,
                'area': area,
                'mean': mean_fit,
                'fwhm': fwhm_fit,
                'temperature': temperature,
                'fit_success': True,
            })

        except (RuntimeError, ValueError):
            # Fallback ohne Fit
            ax0.plot(x_vals, y_vals_plot, color=colors[idx]) # Linienplot der
↪Daten
            area = np.trapezoid(y_vals, x_vals)
            if area < 0: area = abs(area)

            # Rechte Seite Marker
            ax1.scatter(temp_for_plot, area / normalisationfactor,
↪color='black', marker='x')
            peak_metrics.append({
                 'height': np.max(y_vals),
                 'area': area,
                 'mean': x_vals[np.argmax(y_vals)],
                 'fwhm': None,
                 'temperature': temperature,
                 'fit_success': False,
            })

        if peak_metrics[-1]['fit_success']:
```

```
             ax1.scatter(temp_for_plot, area / normalisationfactor, color='black', marker='o')

        temps_for_line.append(temp_for_plot)
        peaks_for_line.append(area / normalisationfactor)

    # Indikator-Balken für Temperatur
    sm = plt.cm.ScalarMappable(cmap=cm.plasma, norm=norm)
    sm.set_array([])
    cbar = plt.colorbar(sm, ax=ax0, orientation='vertical', pad=0.02)
    cbar.set_label('Temperatur in K')

    # Heat/Cool Linien im rechten Plot
    heating_flags = [ht for (_, _, _, ht) in extended_files]
    if True in heating_flags and False in heating_flags:
        split_idx = heating_flags.index(False)
        ax1.plot(temps_for_line[:split_idx], peaks_for_line[:split_idx],
                 color='red', linewidth=1.2, alpha=0.5, zorder=0)
        ax1.plot(temps_for_line[split_idx-1:], peaks_for_line[split_idx-1:],
                 color='blue', linewidth=1.2, alpha=0.5, zorder=0)
    else:
        color = 'red' if all(heating_flags) else 'blue'
        ax1.plot(temps_for_line, peaks_for_line, color=color, linewidth=2, alpha=0.7, zorder=0)

    # Achsenbeschriftungen / Limits
    if plotting.lower() == "energy":
        ax0.set_xlabel('Energie in eV')
        e_min = 1239.84 / x_range[1]
        e_max = 1239.84 / x_range[0]
        ax0.set_xlim(e_min, e_max)
    else:
        ax0.set_xlabel('Wellenlänge in nm')
        ax0.set_xlim(x_range)

    ax0.set_ylim(bottom=0)
    ax1.set_xlabel('Temperatur in K')

    # Y-Labels mit dynamischer Anpassung
    # Linker Plot: Intensität
    if compare and not reference:
        ylabel_0_base = f'Intensität rel. {refmeas}'
    elif reference:
         # Falls es sich selbst um die Referenz handelt
        ylabel_0_base = 'Intensität (arb. u.)'
    else:
        ylabel_0_base = 'Intensität (arb. u.)'
```

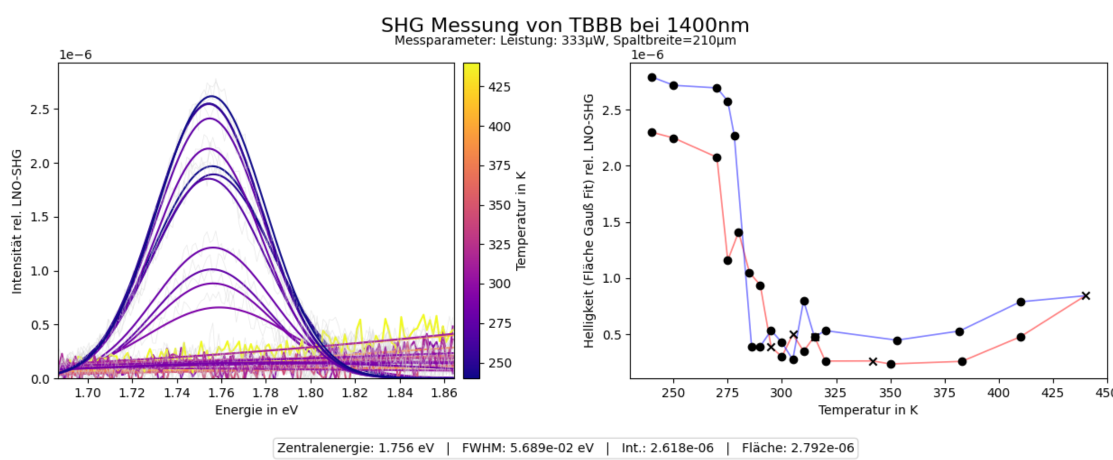
```
    ax0.set_ylabel(ylabel_0_base)

    # Rechter Plot: Fläche
    if compare and not reference:
        ylabel_1_base = f'Helligkeit (Fläche Gauß Fit) rel. {refmeas}'
    else:
        ylabel_1_base = 'Helligkeit (Fläche Gauß Fit) (arb. u.)'

    ax1.set_ylabel(ylabel_1_base)


    fig.suptitle(suptitle, fontsize=16)
    fig.text(0.5, 0.92, f"Messparameter: Leistung: {power}, ␣
↪Spaltbreite={slit_width}", ha="center")

    # Info-Box (Zusammenfassung des besten/höchsten Peaks)
    if len(peak_metrics) > 0:
        best = max(peak_metrics, key=lambda d: d.get('area', float('-inf')))

        # Ausgabe der maximalen unnormierten Fläche
        print(f"Maximale Fläche (unnormiert) der hellsten Messung: {best.
↪get('area'):.16e}")
        print(f"Maximale Intensität (unnormiert) der hellsten Messung: {best.
↪get('height'):.16e}")
        lam0 = best.get('mean', None)
        fwhm = best.get('fwhm', None)
        hoehe = best.get('height', None)
        flaeche = best.get('area', None)

        parts = []
        if lam0 is not None:
            if plotting.lower() == "energy":
                parts.append(f"Zentralenergie: {lam0:.3f} eV")
            else:
                parts.append(f"Zentralwellenlänge: {lam0:.2f} nm")

        if fwhm is not None:
             unit = "eV" if plotting.lower() == "energy" else "nm"
             parts.append(f"FWHM: {fwhm:.3e} {unit}")

        if hoehe is not None:
            val_show = hoehe / norm_intensitaet
            parts.append(f"Int.: {val_show:.3e}")

        if flaeche is not None:
            val_show_area = flaeche / normalisationfactor
```

```
            parts.append(f"Fläche: {val_show_area:.3e}")

        info_text = "   |   ".join(parts) if parts else ""
        if info_text:
            fig.subplots_adjust(bottom=0.18)
            fig.text(0.5, 0.01, info_text, ha='center', va='bottom',
                     fontsize=10,
                     bbox=dict(boxstyle='round', facecolor='white', alpha=0.9,␣
↪edgecolor='lightgray'))

    plt.show()

    # Speichern
    fig.savefig(f'./{filename_prefix}.png', dpi=600, bbox_inches='tight')
    fig.savefig(f'./{filename_prefix}.pdf', dpi=600, bbox_inches='tight')
```

1.2 TBBB

[103]:
```
NLO_plot(
    middle_value=700,
    difference=35,
    filepath='2025-05-22 TBBB/1400nm/0.333mW_Spalt210um/*.asc',
    suptitle='SHG Messung von TBBB bei 1400nm',
    filename_prefix='TBBB_SHG'
)
```

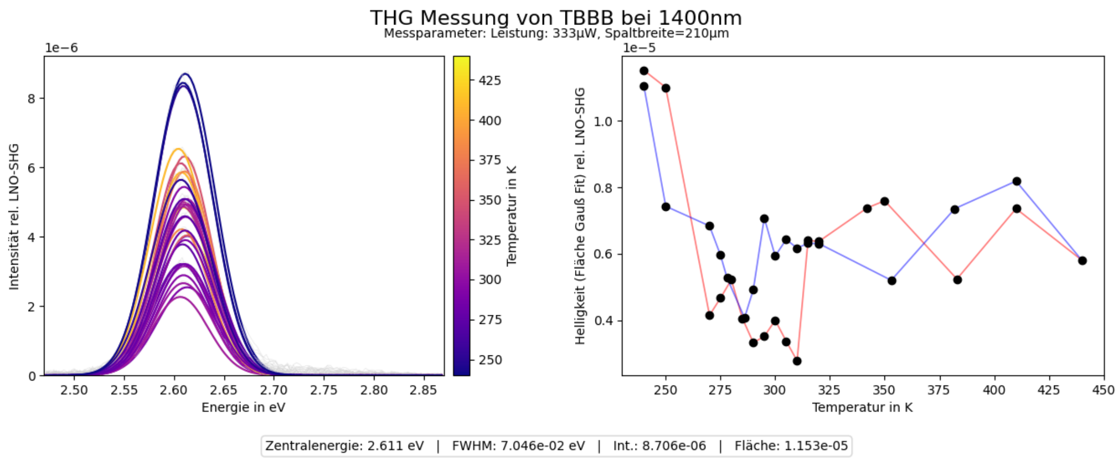
```
Maximale Fläche (unnormiert) der hellsten Messung: 1.0467164796704464e+07
Maximale Intensität (unnormiert) der hellsten Messung: 1.7326693294631448e+08
```



[104]:
```
NLO_plot(
    middle_value=467,
    difference=35,
```

```
    filepath='2025-05-22 TBBB/1400nm/0.333mW_Spalt210um/*.asc',
    suptitle='THG Messung von TBBB bei 1400nm',
    filename_prefix='TBBB_THG'
)
```

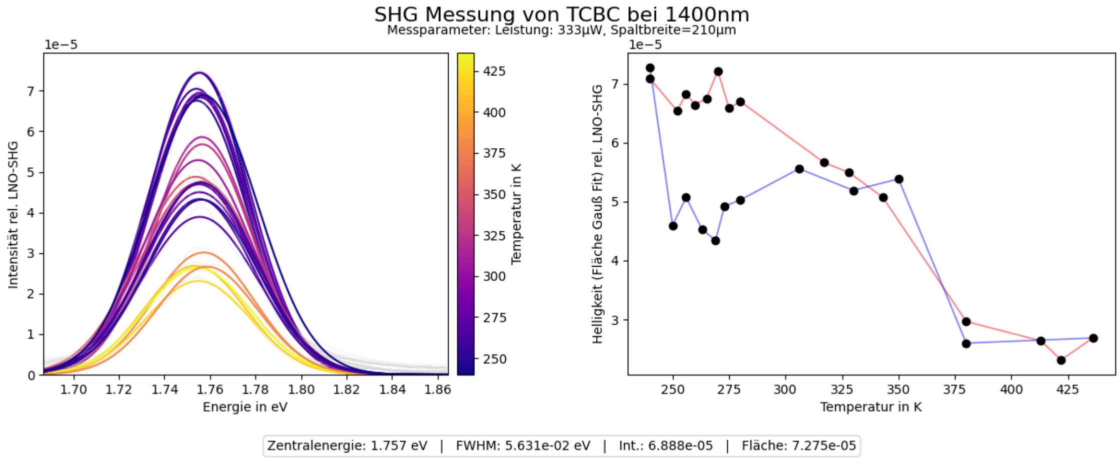
```
Maximale Fläche (unnormiert) der hellsten Messung: 4.3211775144774690e+07
Maximale Intensität (unnormiert) der hellsten Messung: 5.7614813716842008e+08
```



1.3 TCBC

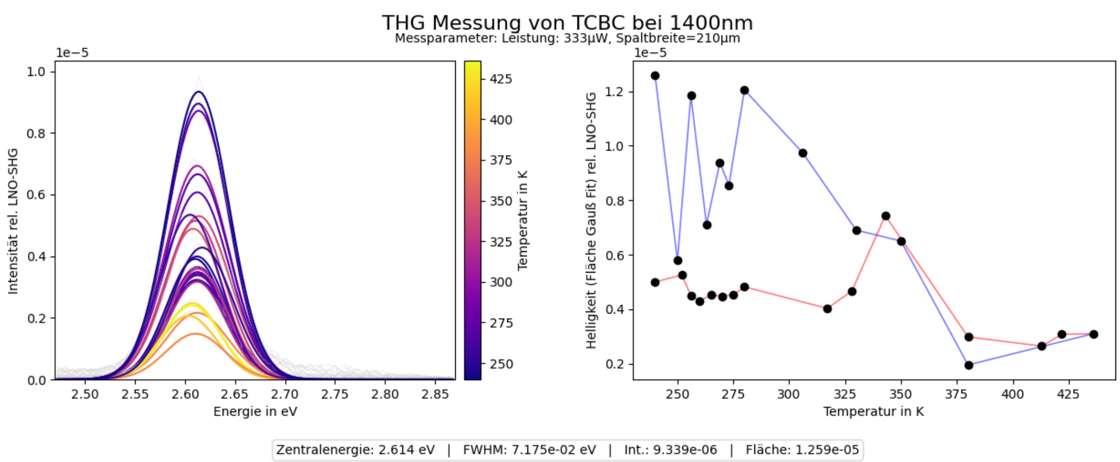
[105]:
```
NLO_plot(
    middle_value=700,
    difference=35,
    filepath='2025-05-23 TCBC/1400nm/0.333mW_Spalt210um/*.asc',
    suptitle='SHG Messung von TCBC bei 1400nm',
    filename_prefix='TCBC_SHG'
)
```

```
Maximale Fläche (unnormiert) der hellsten Messung: 2.7275524845367694e+08
Maximale Intensität (unnormiert) der hellsten Messung: 4.5588114869594164e+09
```




```
[106]: NLO_plot(
    middle_value=467,
    difference=35,
    filepath='2025-05-23 TCBC/1400nm/0.333mW_Spalt210um/*.asc',
    suptitle='THG Messung von TCBC bei 1400nm',
    filename_prefix='TCBC_THG'
)
```

```
Maximale Fläche (unnormiert) der hellsten Messung: 4.7203218375807159e+07
Maximale Intensität (unnormiert) der hellsten Messung: 6.1807786903797257e+08
```



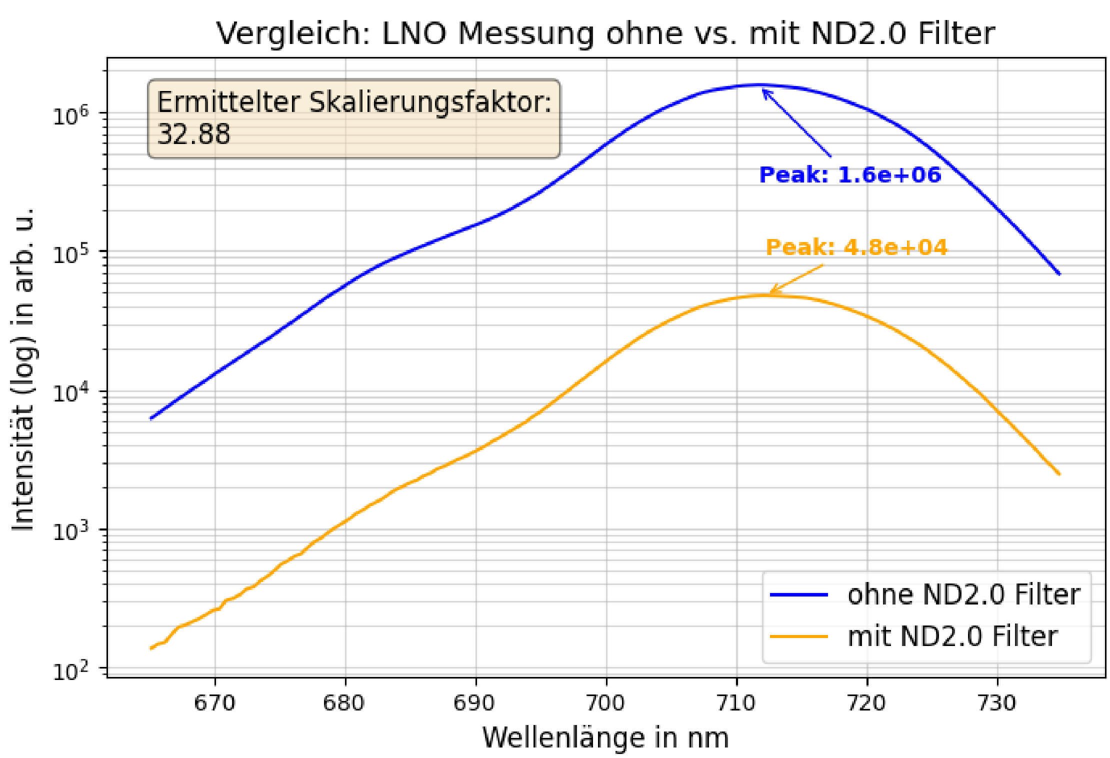
1.4 LNO

Vergleichsmessung

[107]:

```
# Definiere den Wellenlängenbereich wie bei LNO SHG
x_range = (700 - 35, 700 + 35) # anpassen falls verändert!

# Lade die Vergleichsmessungen "mit" und "ohne" ND2.0:
files_ohne = glob.glob('2025-05-23 LNO/1400nm/0.333mW_Spalt210um/Vergleichsmessung ND2.0/ohne*.asc')
files_mit = glob.glob('2025-05-23 LNO/1400nm/0.333mW_Spalt210um/Vergleichsmessung ND2.0/mit*.asc')

# Wähle jeweils die erste Datei (ggf. anpassen, falls mehrere vorhanden)
file_ohne = files_ohne[0]
file_mit = files_mit[0]

# Lade die Daten
freqs_ohne, intensities_ohne = dat2array(file_ohne)
freqs_mit, intensities_mit = dat2array(file_mit)

# Filtere den Bereich wie bei x_range
filtered_data_ohne = [(fr, i) for fr, i in zip(freqs_ohne, intensities_ohne) if x_range[0] <= fr <= x_range[1]]
filtered_data_mit = [(fr, i) for fr, i in zip(freqs_mit, intensities_mit) if x_range[0] <= fr <= x_range[1]]

filtered_freqs_ohne, filtered_intensities_ohne = zip(*filtered_data_ohne) if filtered_data_ohne else ([], [])
filtered_freqs_mit, filtered_intensities_mit = zip(*filtered_data_mit) if filtered_data_mit else ([], [])

# Plotten
fig, ax0 = plt.subplots(figsize=(8, 5))
ax0.plot(filtered_freqs_ohne, filtered_intensities_ohne, label='ohne ND2.0 Filter', color='blue')
ax0.plot(filtered_freqs_mit, filtered_intensities_mit, label='mit ND2.0 Filter', color='orange')

ax0.set_title('Vergleich: LNO Messung ohne vs. mit ND2.0 Filter', fontsize=14)
ax0.set_xlabel('Wellenlänge in nm', fontsize=12)
ax0.set_ylabel('Intensität (log) in arb. u.', fontsize=12)
ax0.set_yscale('log')
ax0.legend(fontsize=12)
ax0.grid(True, which="both", ls="-", alpha=0.5)

peak_ohne = max(filtered_intensities_ohne)
peak_mit = max(filtered_intensities_mit)
peak_ohne_x = filtered_freqs_ohne[filtered_intensities_ohne.index(peak_ohne)]
peak_mit_x = filtered_freqs_mit[filtered_intensities_mit.index(peak_mit)]
```

```
# Berechne den Skalierungsfaktor
skalierungsfaktor = peak_ohne / peak_mit

ax0.annotate(f'Peak: {peak_ohne:.1e}', xy=(peak_ohne_x, peak_ohne),␣
 ↪xytext=(peak_ohne_x, peak_ohne*0.2),
             arrowprops=dict(arrowstyle='->', color='blue'), color='blue',␣
 ↪fontsize=10, fontweight='bold')
ax0.annotate(f'Peak: {peak_mit:.1e}', xy=(peak_mit_x, peak_mit),␣
 ↪xytext=(peak_mit_x, peak_mit*2),
             arrowprops=dict(arrowstyle='->', color='orange'), color='orange',␣
 ↪fontsize=10, fontweight='bold')

# Faktor deutlich im Plot anzeigen
textstr = f'Ermittelter Skalierungsfaktor:\n{skalierungsfaktor:.2f}'
props = dict(boxstyle='round', facecolor='wheat', alpha=0.5)
ax0.text(0.05, 0.95, textstr, transform=ax0.transAxes, fontsize=12,
        verticalalignment='top', bbox=props)

# plt.tight_layout()
plt.show()

print(f"Skalierungsfaktor (ohne ND2.0 / mit ND2.0): {skalierungsfaktor:.2f}")
```

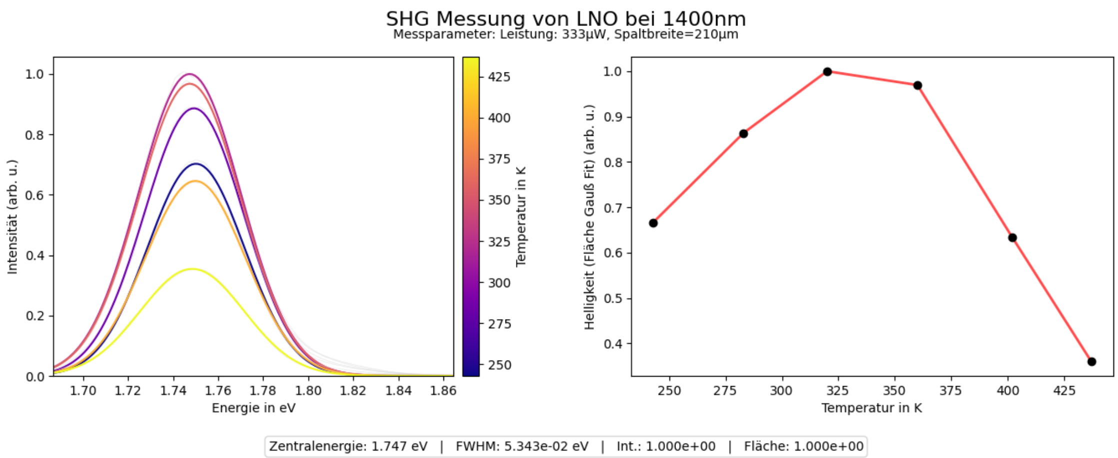


Skalierungsfaktor (ohne ND2.0 / mit ND2.0): 32.88

1.4.1 SHG

[108]:
```
NLO_plot(
    middle_value=700,
    difference=35,
    filepath='2025-05-23 LNO/1400nm/0.333mW_Spalt210um/*.asc',
    suptitle='SHG Messung von LNO bei 1400nm',
    filename_prefix='LNO_SHG',
    reference=True
)
```

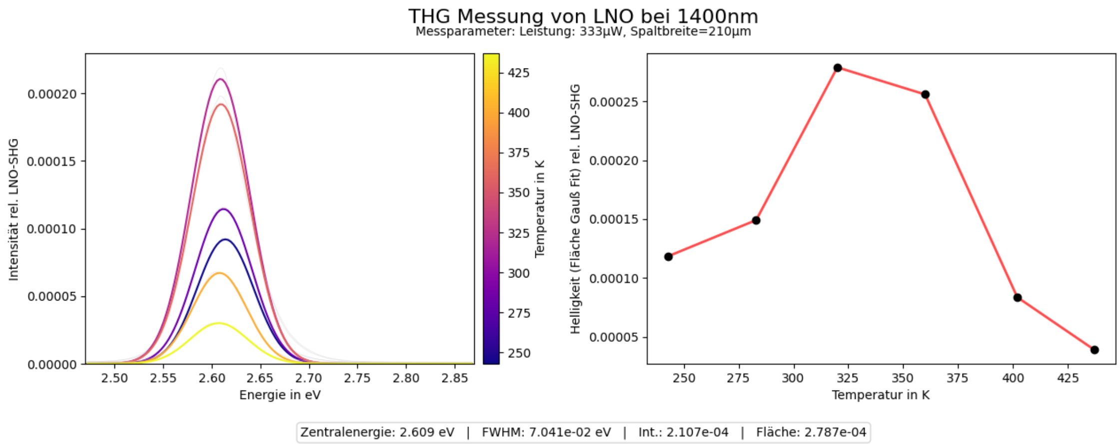
Maximale Fläche (unnormiert) der hellsten Messung: 3.7490887328811729e+12
Maximale Intensität (unnormiert) der hellsten Messung: 6.6181976473128055e+13



1.4.2 THG

[109]:
```
NLO_plot(
    middle_value=467,
    difference=35,
    filepath='2025-05-23 LNO/1400nm/0.333mW_Spalt210um/*.asc',
    suptitle='THG Messung von LNO bei 1400nm',
    filename_prefix='LNO_THG'
)
```

Maximale Fläche (unnormiert) der hellsten Messung: 1.0449557815527937e+09
Maximale Intensität (unnormiert) der hellsten Messung: 1.3942079737029299e+10

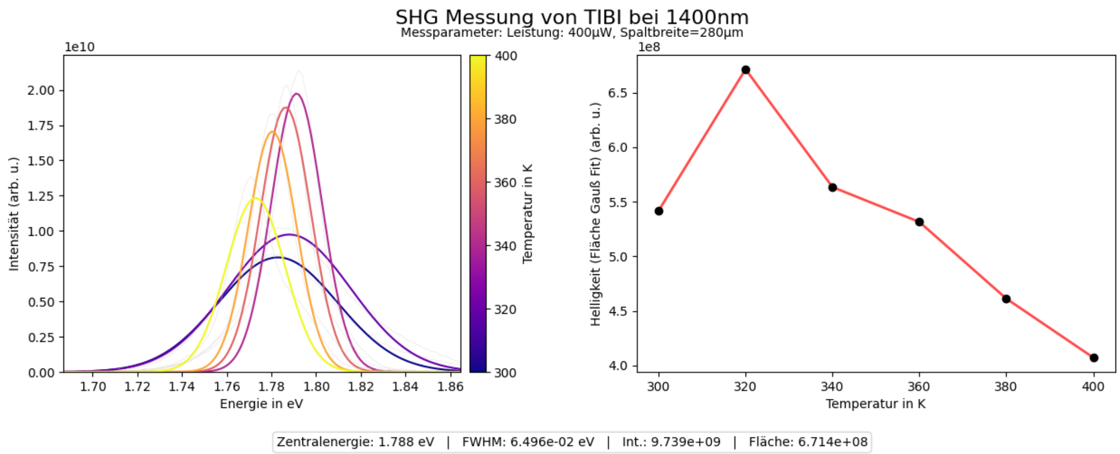


1.5 TIBI

1.5.1 SHG

[110]:
```
NLO_plot(
    middle_value=700,
    difference=35,
    filepath='TIBI_400uW_1400nm/*.asc',
    suptitle='SHG Messung von TIBI bei 1400nm',
    filename_prefix='TIBI_SHG',
    power="400µW",
    slit_width="280µm",
    compare=False,
    reference=False,
    normalisationfactor=1,
    norm_intensitaet=1,
)
```

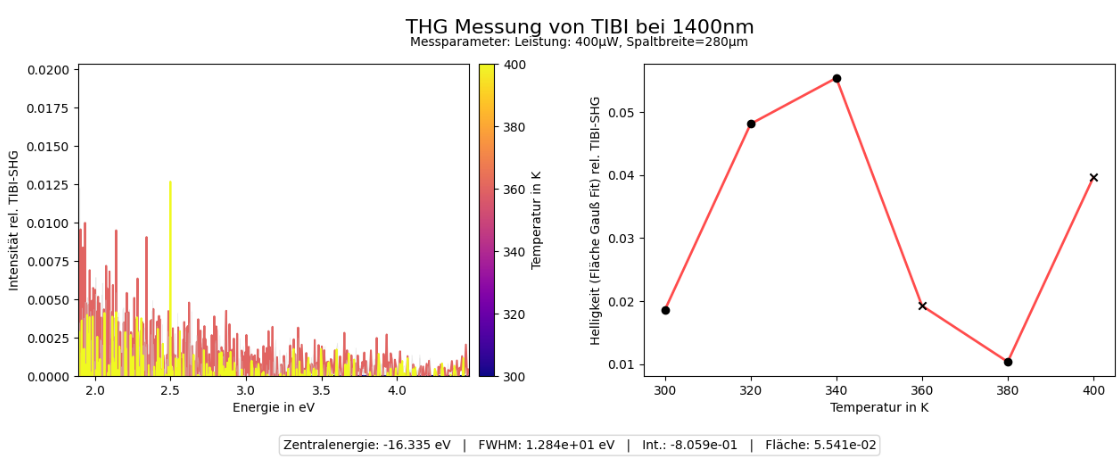
```
Maximale Fläche (unnormiert) der hellsten Messung: 6.7143405906491041e+08
Maximale Intensität (unnormiert) der hellsten Messung: 9.7393162937730503e+09
```



1.5.2 THG

[111]:
```
NLO_plot(
    middle_value=467,
    difference=190,
    filepath='TIBI_400uW_1400nm/*.asc',
    suptitle='THG Messung von TIBI bei 1400nm',
    filename_prefix='TIBI_THG',
    power="400µW",
    slit_width="280µm",
    compare=True,
    normalisationfactor=6.7143405906491041e+08,
    norm_intensitaet=9.7393162937730503e+09,
    refmeas="TIBI-SHG"
)
```

```
Maximale Fläche (unnormiert) der hellsten Messung: 3.7206094658960387e+07
Maximale Intensität (unnormiert) der hellsten Messung: -7.8489996324543819e+09
```

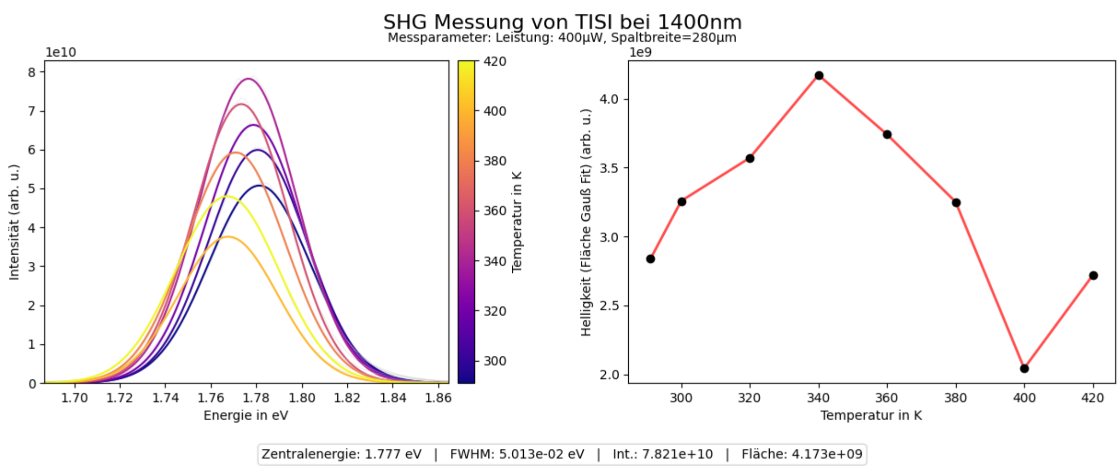


1.6 TISI

1.6.1 SHG

[112]:
```
NLO_plot(
    middle_value=700,
    difference=35,
    filepath='TISI_400uW_1400nm/*.asc',
    suptitle='SHG Messung von TISI bei 1400nm',
    filename_prefix='TISI_SHG',
    power="400µW",
    slit_width="280µm",
    compare=False,
    reference=False,
    normalisationfactor=1,
    norm_intensitaet=1
)
```

```
Maximale Fläche (unnormiert) der hellsten Messung: 4.1730454418659124e+09
Maximale Intensität (unnormiert) der hellsten Messung: 7.8205974134100433e+10
```



1.6.2 THG

[113]:
```
NLO_plot(
    middle_value=467,
    difference=190,
    filepath='TISI_400uW_1400nm/*.asc',
    suptitle='THG Messung von TISI bei 1400nm',
    filename_prefix='TISI_THG',
```

```
    power="400µW",
    slit_width="280µm",
    compare=True,
    normalisationfactor=4.1730454418659124e+09,
    norm_intensitaet=7.8205974134100433e+10,
    refmeas="TISI-SHG"
)
```

```
Maximale Fläche (unnormiert) der hellsten Messung: 3.2116164198759556e+07
Maximale Intensität (unnormiert) der hellsten Messung: 1.6168114967745182e+08
```