# Molecular Vibration Explorer

**Molecular Vibration Explorer** is an interactive tool for exploring molecular vibrational spectra and tensorial light-vibration coupling strength for applications in the field of surface-enhanced spectroscopy. The **Gold** database gathers the results from density functional theory calculations on 2’800 commercially available thiol compounds linked to a gold atom, with the main motivation to screen the best molecules for THz and mid-infrared to visible upconversion, as reported in Ref. [1]. The **Thiol** database contains calculations on 1’900 commercially available thiol compounds. The different tools available to analyze the database were previously introduced in Ref. [1,2].
Spectroscopies:

- Infrared absorption
- Raman scattering
- Infrared to Raman conversion / vibrational sum-frequency generation

Functionalities:

- Molecular screening based on intensity of individual normal modes or in a spectral window
- Electromagnetic field polarization directions
- Random or specific molecular orientation wrt. polarization vectors

References:


- [1] Z. Koczor-Benda, A. L. Boehmke, A. Xomalis, R. Arul, C. Readman, J. J. Baumberg & E. Rosta "Molecular Screening for Terahertz Detection with Machine-Learning-Based Methods", *Phys. Rev. X* **11**(4):041035 (2021)
- [2] P. Roelli, D. Martin-Cano, T.J. Kippenberg & C. Galland, "Molecular Platform for Frequency Upconversion at the Single-Photon Level", *Phys. Rev. X*, **10**(3):031057 (2020)