Computing Molecular Vibrations with ASAP

Diverse applications in various scientific fields, ranging from chemistry and physics to materials science and biology:

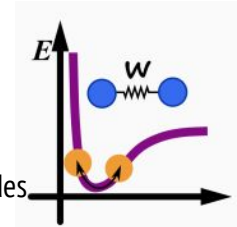
ASAP provides an user-friendly workflow for studying molecular vibrations,

Input:

- Geometric structure

Output:

- Vibration modes
- Density of vibration modes



Method: Finite difference approximation of the Hessian matrix.

- SPECTROSCOPY. Interpreting spectroscopic techniques (such as IR and Raman).
- CATALYSIS. Understanding the vibrational modes of reactants, intermediates and products is crucial in studying catalytic reactions.
- DRUG DESIGN. Understanding the vibrational modes helps in predicting bioactivity, drug-receptor interactions and the stability of drug compounds.
- BIOCHEMISTRY. Providing insights into molecular vibrations involved in biological processes.

Case Study: Designing molecular nanosensors

Developing high-resolution molecular biosensors from an enhanced infrared absorption spectrum* (Multiscale Approach)

Simulation of the vibrational spectra for the conformational states of the target proteins (DFT with ASAP)

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Metallic antenna design. The geometric dimension of the antennas is defined through calculations of the electromagnetic response of the nanostructures (finite element method with COMSOL).

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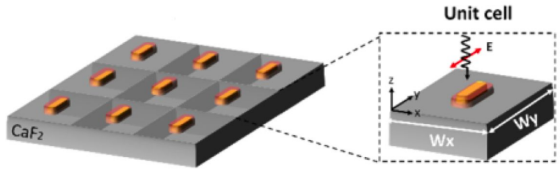
Antenna fabrication design and characterization



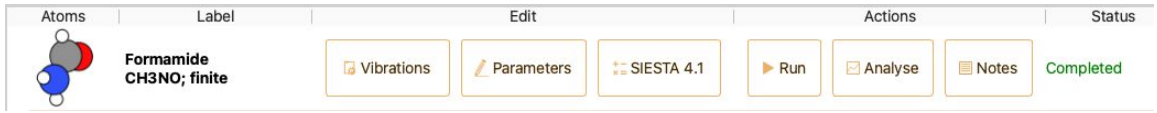
Schematic representation of the set up used to study the electromagnetic response of the antenna in the presence of the target protein. It is considered that the antenna is interacting with a distribution of proteins representing a conformal layer. (Figure provided by Mario Zapata -Materials Physics Center-.

*Project funded by The Provincial Council of Gipuzkoa, call "Gipuzkoa Quantum-2022" / Project partners: Atten2 Advanced Monitoring Technologies, Tekniker and Simune.

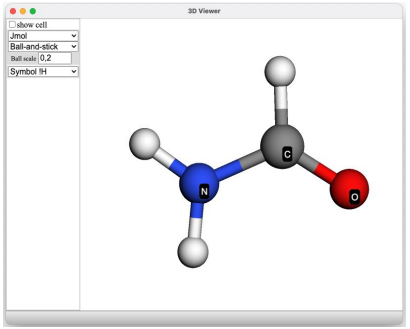
The project results are confidencial.
The following slides provide simulations of the vibrational spectra for the selected reference molecule in this study: Formamide (CH_3NO)

Case Study: Designing molecular nanosensors

Identification of the frequencies that characterize the protein Formamide (CH_3NO) (reference molecule)

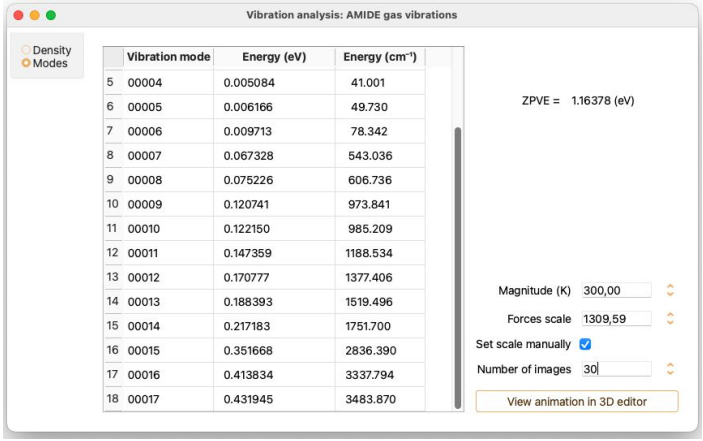


ASAP[1] constructed ball-and-stick model representation of the atomistic structure of formamide (CH_3NO).



[1] ASAP (Atomistic Simulation Advanced Platform) https://www.simuneatomistics.com/services/asap-software/

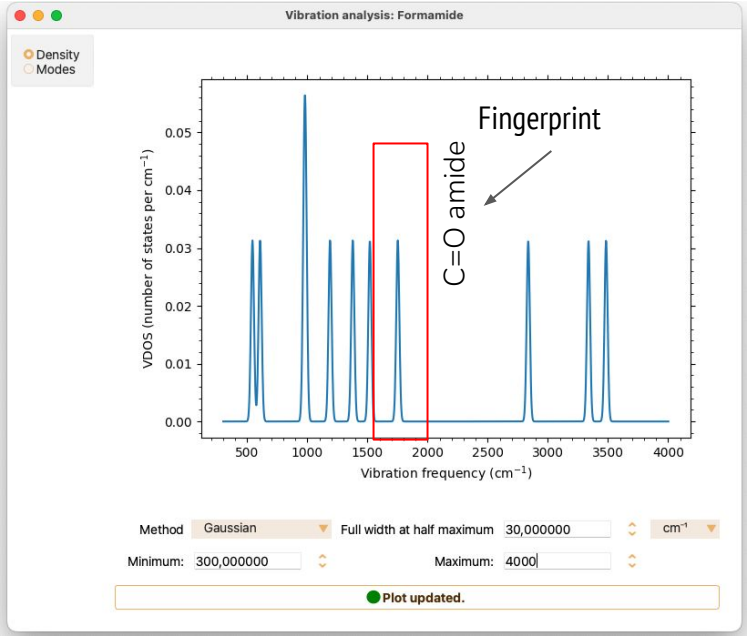
ASAP analysis window showing the computed absorption frequencies of CH_3NO (in vacuum).



The results are in good agreement with the frequencies obtained by Sugawara et al.[2] using Fourier-transform infrared spectroscopy. [2]Sugawara, Y.; Hamada, Y. y Tsuboi, M., Vibration-rotation Spectra of Formamides, Bulletin of the Chemical Society of Japan, 56, 1045-1050 (1983).

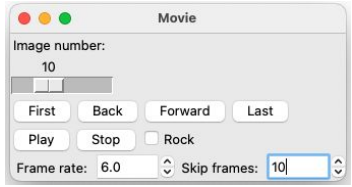
Case Study: Designing molecular nanosensors

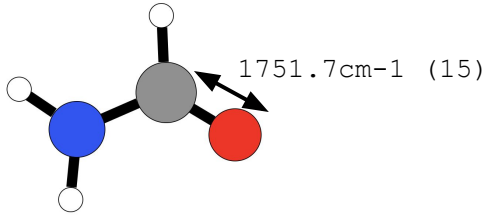
ASAP analysis window showing the density of vibrational modes of CH_3NO (in vacuum)



The calculations were repeated in water solvent (implicit model). We observe that the C=O amide peak decreases by 48.1 cm^{-1}.

ASAP allows to visualise the animation of the selected vibrational mode





CONCLUSIONS

ASAP/SIESTA provides an user-friendly workflow for the exploration of molecular vibrations.

Formamide (CH_3NO) was chosen as the reference molecule, serving as a benchmark for method precision calibration. Our investigation seamlessly extended to a target protein (*confidential*).

This study provides crucial guidelines for the strategic design of nanoscale antennas. Antennas are engineered to enable frequency coupling between molecular vibrations and the dipolar resonance of the antennas.