Computational physics use case

This use case described a research task that focused on testing the Schrödinger API, a thematic service, using the FINKI Cloud service, which is fully onboarded on the NI4OS-Europe service catalogue. The researchers asked users to report their answers to questions related to Jupyter notebooks and the usefulness of the Schrödinger API. Additionally, the researchers were asked to report any technical difficulties they faced while using the services.

The use case also discussed the use of infrared multiple photon dissociation (IRMPD) spectroscopic techniques in exploring size-selected species in detail.

The following actions were taken:

- The task focused on testing the Schrödinger API using the FINKI Cloud.
- Jupyter notebooks were used in this research.
- The researchers asked users about their experience with Jupyter notebooks and the usefulness of the Schrödinger API.
- The majority of researchers found Jupyter notebooks and the Schrödinger API useful.
- The researchers did not report any major technical difficulties with the services.
- Infrared multiple photon dissociation (IRMPD) spectroscopic techniques were used to explore size-selected species in detail.

For more information about the use case please visit the NI4OS-Europe training platform, as well as the submitted deliverable 6.4.