SSHADE, the European solid spectroscopy database infrastructure

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The SSHADE database infrastructure (http://www.sshade.eu) hosts spectral data from many different types of materials: minerals, meteorites, organic matters, …, as well as calculated spectra, covering the whole electromagnetic spectra from gamma rays to radio wavelengths. Its searching / viewing / downloading interface is operational and open to users since February 2018. The SSHADE consortium currently gathers 21 laboratories from 11 different countries.

In this context, the ESRF FAME et FAME-UHD beamlines have joined SSHADE by creating the SSHADE/FAME database. Two main goals motivated this initiative:
- filling the lack of XAS databases. Indeed, few databases exist in the domain and they generally provide too few details in the sample descriptions, so that it is difficult to use the spectra for data analysis. The consequences are a multiplication of measurements on identical samples across the different beamlines, and a lack of global complementarity between beamlines, generating a global waste of beam time.
- anticipating the current political trend which requires to render all the data publicly available, but also making these data effectively accessible, reusable, indexed and containing enough details to build a repository that could be used in the future for simulation codes (e.g. based on artificial intelligence).

Being part of SSHADE, the SSHADE/FAME database is a durable solution (its has been labeled by the CNRS/INSU as a National Observation Service). It is based on an elaborate data model which enables a very precise description of all the elements (from the sample to the measurement) and an efficient and user-friendly search strategy. Moreover, by attributing a DOI (Digital Object Identifier) to each data set, it offers the possibility to diffuse the spectra in a robust way and accordingly to the current publication recommendations. The database already contains more than 200 XAS spectra (and more than 1800 spectra in total).

The poster will present the database, its goals, its specificities and its use, from both the spectra user and provider points of view.