Labex MATISSE

Axe

Probing the quantum thermal fluctuations of nuclei by XANES and NMR spectroscopy

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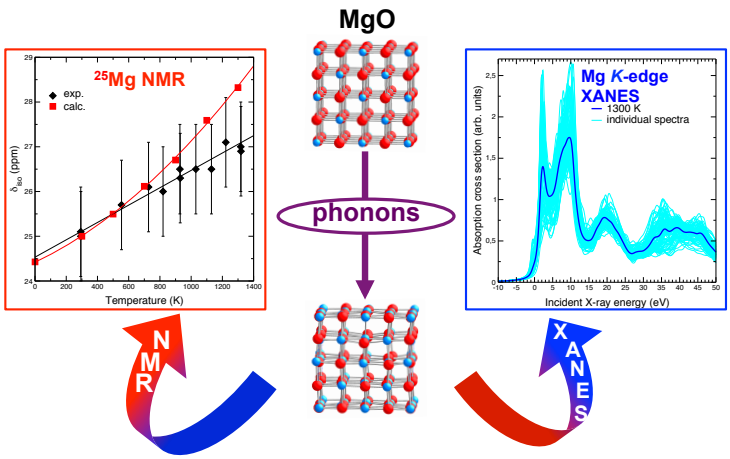

Effets des fluctuations thermiques quantiques des noyaux atomiques dans le cas de MgO. Les vibrations déplacent sensiblement les noyaux atomiques de leurs positions d'équilibres, modifiant ainsi la structure cristallographique bien connue aux courtes échelles de temps. Ceci provoque des variations remarquables des spectres d'absorption X (XANES) et sur les paramètres RMN

Hosting laboratories, teams and and thesis supervisors names:

Institut de Minéralogie ; Physique des Matériaux et Cosmochimie – Équipe TQM – Delphine Cabaret
Laboratoire de Chimie de la Matière Condensée de Paris – Équipe SMILES – Christel Gervais

Research project

Electronic structure calculations are performed considering the nuclei fixed to their equilibrium positions. However, the atoms perpetually move due to thermal quantum fluctuations even at absolute zero. Furthermore, these variations significantly affects the spectroscopic data. In X-ray Absorption Spectroscopy (XANES), particularly at the *K*-edges of light elements in oxides, we observe the emergence and evolution with temperature of fine structures corresponding to electronic transitions forbidden by symmetry. In the case of Nuclear Magnetic Resonance (NMR), chemical shifts remarkably vary with temperature. The purpose of this project is: (i) experimentally observe these effects in different reference compounds, (ii) describe the theory by developing an original method based on DFT, taking into account harmonic and anharmonic fluctuations of nuclei.

Scientific results & impacts

We obtained high-quality experimental data in NMR and XANES at different temperatures in various oxides, that we are now able to reproduce. We thouroughly studied the case of MgO and highlighted the importance of the vibrations of quantum origin under the quasi-harmonic approximation. We extend this experiment-calculation combined approach to structurally more complex oxides such as $AlPO_4$, Al_2O_3, $SiAl_2O_5$.

Main key facts (for instance publications / pri ces / oral presentations)

Publication in preparation for an international peer-reviewed journal.
4 oral communications in international conferences: LUCIA a 10 ans, JEELS2014, ICAMM2014 & JMC14-CMD25
1 poster: SOLEIL User's Meeting 2014