# Thesis Project Offer

*Joint Research and Education Programme "Palestinian-German Science Bridge PGSB"*
*Forschungszentrum Jülich GmbH & Palestine Academy for Science and Technology*

## Thesis type*

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| ☐ BSc | ☒ MSc | ☐ PhD | Intended starting date (approx.): As soon as possible |

## Contact details of supervisor/responsible host at Forschungszentrum Jülich


| Title* | Degree | First name* | Surname* |
|---|---|---|---|
| Ms.<br>Mr. | Dr.<br>Prof. | Sabreen<br>Manuel | Hammouda<br>Angst |

| Phone* | E-mail* |
|---|---|
| +49 89/158860-744 | **s.hammouda@fz-juelich.de** |

| Function* | Institute and homepage of institute* |
|---|---|
| **Postdoctoral researcher** | **JCNS-4 and JCNS-2** |

| University affiliation in Germany* |
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## Co-Supervisor at Palestinian university (if applicable)

| Title | Degree | First name | Surname |
|---|---|---|---|
| Title | Degree | | |

| Phone | E-mail |
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| University/institution | Department/faculty/institute |
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## Project description*

**Elucidation of the charge order of $Lu_3Fe_4O_{10}$**

The rare earth ferrite $LuFe_2O_4$ attracted attention due to a proposed, though not confirmed, ferroelectricity arising from charge ordering (CO) in Fe/O bilayers [1,2], a novel mechanism to obtain multiferroic materials for potential applications in information technology. It would be of high interest to elucidate the evolution of charge order upon intercalation, i.e. the insertion of one or several $LuFeO_3$ block(s) between the bilayers in $LuFe_2O_4$, modifying their coupling and making a polar CO more likely.

During the growth of the first intercalated compound $Lu_2Fe_3O_7$, an intergrowth of the second intercalated compound $Lu_3Fe_4O_{10}$ occurred and crystals were stoichiometric enough to exhibit a 3D charge order were obtained as a second phase [3]. The performed macroscopic magnetization measurements on those crystals indicate a sharp transition in contrast to the $Lu_2Fe_3O_7$ compound [3,4,5]. Furthermore, based on the observed propagation vector, the representation analysis indicates that this compound is very likely polar. Therefore, studying the $Lu_3Fe_4O_{10}$ compound is very fruitful.

Achieving the aim of elucidating the CO of $Lu_3Fe_4O_{10}$ requires the fabrication of a sample in the form of single crystals. For this, polycrystalline samples need to be synthesized first.

The most critical aspect of such a study is the oxygen stoichiometry needs to be fine-tuned, as otherwise, changes are impossible to cleanly disentangle from the intercalation. The synthesis of polycrystalline samples therefore should be done under a $CO_2$-$H_2$ (4%)/Ar (96%) gas flow, and single crystals should be grown in an image furnace under a tunable flow of CO: $CO_2$ to control the oxygen partial pressure.

The fellow will characterize the samples by X-ray powder diffraction to check the phase purity, and by low-field magnetization to indicate the stoichiometry. The characterization results will be used as feedback to optimize the synthesis parameters. The charge order can then be investigated by single-crystal x-ray diffraction at the synchrotron after screening many crystals with in-house single-crystal diffractometer.

**The fellow should have a physics or material science background.

References:

[1] N. Ikeda et al., Ferroelectricity from iron valence ordering in the charge-frustrated system $LuFe_2O_4$, Nature 436, 1136–1138 (2005).
[2] M. Angst, Ferroelectricity from iron valence ordering in rare earth ferrites?, Phys. Status Solidi RRL 7, 375 (2013).
[3] S. Hammouda and M. Angst, Growth of layered $Lu_2Fe_3O_7$ and $Lu_3Fe_4O_{10}$ single crystals exhibiting long-range charge order via the optical floating-zone method, J.Cryst. Growth 521, 50 (2019).
[4] S. Hammouda et al., Magnetic properties of the intercalated compound Lu2Fe3O7, Phys. Rev. B 104, 174437 (2021).
[5] S. Hammouda, PHD thesis, RWTH Aachen University (2021).

| Date* | Signature* |
|---|---|
| 23.01.2023 | Sabreen Hammouda |

* required field