CSC-RUB PhD Project Proposal

Title: Ferroelectric phase diagrams and functional properties of hybrid ferroelectrics

Sector of research: Materials Science / Condensed Matter Physics

Degree awarded: PhD or Dr.rer.nat.

Keywords: ferroelectrics, hybrid perovskites, density functional theory, molecular dynamics simulations, phase diagrams, functional response

Supervisors of PhD project:

Prof. Dr. Anna Grünebohm

Email: anna.gruenebohm@rub.de; ORCID: 0000-0001-9299-058X

Ralf Drautz, Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-University Bochum

Research focus of supervisor:

Me and my group we utilize and develop scale-bridging simulation methods to fundamentally understand and optimize ferroelectric materials for energy applications. In particular we focus on the coupling between microstructure (domain and defect structures, interfaces, and inhomogeneities in solid solutions) and functional responses (piezoelectric, dielectric electrocaloric responses).

I am leading the Emmy-Noether group "Scale-bridging computational design of multifunctional ferroelectric composites" funded by the German Research foundation and my work in the field of electrocaloric has been awarded by the Innovation price of the state NRW 2020.

Publications:

So far, I published more than 30 papers (H index: 13) in refereed journals such as Phys. Rev. B, Appl. Phys. Lett., or Appl. Phys. Rev.:

1) **A. Grünebohm** and M. Marathe, *Impact of domains on the orthorhombic-tetragonal transition of* $BaTiO_3$*: An ab initio study*,
Phys. Rev. Materials 4, 114417 (2020).

2) A. S. Everhardt, T. Denneulin, **A. Grünebohm**, Y.-T. Shao, P. Ondrejkovic, S. Zhou, N. Domingo, G. Catalan, J. Hlinka, J.-M. Zuo, S. Matzen and B. Noheda, *Temperature-independent giant dielectric response in transitional* $BaTiO_3$ *thin films*, Appl. Phys. Rev. 7, 011402 (2020).

3) **A. Grünebohm**, Y.-B. Ma, M. Marathe, B.-X. Xu, K. Albe, C. Kalcher, K.-C. Meyer, V. V. Shvartsman, D. C. Lupascu and C. Ederer, *Origins of the inverse electrocaloric effect, Energy Technol.* 6, 1491 (2018).

4) **A. Grünebohm** and T. Nishimatsu, *Influence of defects on ferroelectric and electrocaloric properties of* $BaTiO_3$, Phys. Rev. B 93, 134101 (2016).

5) M. Marathe, **A. Grünebohm**, T. Nishimatsu, P. Entel and C. Ederer, *First-principles-based calculation of the electrocaloric effect in* $BaTiO_3$*: comparison of direct and indirect methods*,

Phys. Rev. B 93, 054110 (2016).

Summary of research plan

Background: Ferroelectric materials are widely used in applications and are promising for energy harvesting devices as well as for future efficient solid-state cooling devices based on the electrocaloric effect. All these applications share the following demands on materials design: Replace toxic Pb and increase efficiency and reversibility in a broad and suitable operation range. Despite their obvious advantages (light weight, flexible, easy to produce) the ferroelectric und functional properties of hybrid perovskites such as ($Me_3NCH_2XN^+$) TM Y_3 (with X, Y: Cl, Br, I and TM=Fe,Mn) are often neglected in this quest and even their fundamental understanding is incomplete.

Study objective: The goals of the project are an improved fundamental understanding of ferroelectric and related functional properties of hybrid perovskites and the generation of composition-temperature phase diagrams as starting point for a targeted material optimization.

Expected Results:
The improved understanding of the coupling between complex atomic structure, energy landscapes and phase stability in hybrid ferroelectrics is not only of fundamental interest but important to judge the technological potential of these materials for different applications and to narrow down the range of optimal constituents. The outcome of these study will be published in international peer-reviewed journals and will be directly linked to experimental work at the nearby university of Duisburg-Essen.

Methods: Molecular dynamics simulations (LAMMPS);
DFT simulations (abinit and/or VASP code) on the high performance computer at RUB.

Candidate Requirements:

- an excellent master's degree in materials science or condensed matter physics
- a high level of spoken and written English (IELTS band score of 6.5 or higher)
- strong background in MD simulations
- high motivation to collaborate in an international interdisciplinary team

Motivation for CSC application:

The successful candidate will be working in the new research centre for interface-dominated high-performance materials (ZGH) at Ruhr University Bochum, providing an excellent working environment and access to the supercomputer at RUB. The PhD candidate will be member of a highly motivated young group which closely collaborates with experts on method development and ferroelectrics at RUB (within the material research department and the interdisciplinary centre of advanced materials simulation), in the nearby area (Uni Duisburg-Essen) and all over the world (in particular ETH Zürich).

All PhD students at ICAMS benefit from the soft skill classes offered by the Ruhr University Research School and are members of the Graduate School “Scale-Bridging materials modelling” (http://www.icams.de/content/icams-graduate-school/).