CSC-RUB PhD Project Proposal

Title: Functional properties of ferroelectric superlattices: an *ab initio* based scale-bridging study on $BaTiO_3$/$Ba(Ti,Sn)O_3$

Sector of research: Materials Science / Condensed Matter Physics

Degree awarded: PhD or Dr.rer.nat.

Keywords: ferroelectrics, superlattices, density functional theory, molecular dynamics simulations, domain structure, phase diagrams, strain engineering, functional response

Supervisor of PhD project: Prof. Dr. Anna Grünebohm, e-mail: anna.gruenebohm@rub.de

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) T. Nishimatsu, **A. Grünebohm**, U. Waghmare and M. Kubo, *Molecular Dynamics Simulations of Chemically Disordered Ferroelectrics $(Ba,Sr)TiO_3$ with a semi-empirical effective Hamiltonian*, J. Phys. Soc. Jpn. 85, 114714 (2016).

Summary of research plan

Background: Ferroelectric perovskites 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. Extensive work on $BaTiO_3/SrTiO_3$ in the last years revealed exceptional functional responses and exotic domain patterns for superlattices made of ferroelectric and paraelectric materials. So far, systematic studies on superlattices with other constituents are rare least equally promising for applications.

Study objective: The goal of the project is the fundamental understanding of the domain structure and the resulting functional responses of superlattices of $BaTiO_3/Ba(Sn,Ti)O_3$.

Expected Results:
Method: We will validate and improve scale-bridging simulation methods for of $Ba(Sn,Ti)O_3$ which will be the starting point for further studies in the future.
Material: We will reveal the phase diagram and domain structure of $BaTiO_3/Ba(Sn,Ti)O_3$ superlattices and communicate our results on international conferences and publish in high-ranked journals. The important question to be answered is: Are functional response and domain structure in Sn-concentration graded superlattices similar or even superior to $BaTiO_3/SrTiO_3$? This work will contribute to the systematic understanding of ferroelectric superlattices.

Methods: Molecular dynamics simulations (LAMMPS and open-source code feram);
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 DFT and/or MD simulations and python coding
- 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/).