

**Jan Barański @ Max Planck Institute for Solid State Research, Stuttgart, Germany**



From 29.02.2016 till 04.03.2016 I was visiting Max Planck Institute for Solid State Research in Stuttgart. Under supervision of professor Anette Bussmann-Holder I improved my abilities on performing theoretical calculations on perovskite structure ferroelectrics. The co-workers from our department perform experiments on such compounds and so, suitable theoretical treatment was highly desirable. First, we discussed the details of a polarizability model. This treatment involves analytical methods supported by experimental data. The main task was to calculate dispersion relations for, so-called, “soft-modes”. These modes are believed to be responsible for occurrence of ferroelectricity in oxygen compounds. One of the problems solved was how to fit the model parameters to experimental data of a given compound and implement them to the self-consistent calculations. After discussion on the applications and limitations of the model we turned to numerical calculations. I was running a program, which self consistently calculates the dispersion relation of a given compound. In particular, after some instructions I was able to reproduce previous results for  $\text{SrTiO}_3$  and  $\text{KTaO}_3$  analysed in [1]. Calculations for these exemplary compounds prove that the program works correctly, and I will be able to work on more sophisticated problems on my own. Lastly we discussed the recent development of oxide-based ferroelectrics and possible paths for new researches. We were mostly concerned about the multiferroic materials like  $\text{EuTiO}_3$ , which exhibit more than one type of ferroic ordering.

My visit to Max Planck Institute was very satisfying, due to friendly environment, and very fruitful, as I significantly improved my skills in theory of oxide-based ferroelectrics and was instructed on recent developments concerning the issues of great interest to me. Finally thanks to ERASMUS programme I developed new relationships with MPI workers. I would like to thank prof. Annette Bussmann Holder and dr Reinhard K. Kremer for assistance during my stay at MPI Stuttgart.

[1] A.Bussmann-Holder J. Phys.: Condens. Matter 24 (2012) 273202