Ing. Pavel Márton, Ph.D. – Curriculum Vitae 2023

Born: 12.07.1979 in Liberec, Czech Republic

Affiliations: **Institute of Physics, Academy of Sciences of the Czech Republic (ASCR)**, *Na Slovance 2, 182 21 Praha, Czech Republic,* +420 266 052 126 marton@fzu.cz

Institute of Mechatronics and Computer Engineering, Technical University of Liberec (TUL), *Studentská 2, 46117 Liberec, Czech Republic,* +420 485 353 738 pavel.marton@tul.cz

Researcher ID: G-1611-2011

Scopus: 57205889974

ORCID: 0000-0001-7273-7288

Academic background

2003-2007 **Charles University in Prague, Faculty of Mathematics and Physics,** *Ke Karlovu 3, 121 116 Praha, Czech Republic,* Ph.D. studies, **specialization: mathematical modeling,** doctoral thesis defended in 2007

1998-2003 **Czech Technical University in Prague, Faculty of Nuclear Science and Physical Engineering,** *Břehová 7, 115 19 Praha, Czech Republic,* **specialization: software engineering,** master degree received in 2003

Work experience and research areas

10.2010-now **Institute of Physics ASCR, Department of dielectrics**

2018-now serving as the **head of the Theory and simulations group**

Topics: theoretical study of ferroelectric and multiferroic materials, domain structure theory, ab-initio, atomic-level, phase-field simulations and calculations, development of parametrizations for models based on first-principles calculations

01.2011-now **Faculty of Mechatronics Informatics and Interdisciplinary Studies, Institute of Mechatronics and Computer Engineering, TUL**

Topics: Piezoelectric materials for applications, vibration damping using active-elasticity constrol, energy harvesting, computational chemistry, programming of a computer package **ferrodo** for simulations of formation and evolution of domain structures in ferroelectrics

Teaching: Lecturer of courses: Quantum mechanics 1, Quantum physics of solids, Electromagnetism and optics

Supervisor of 1 doctoral student (defended 2016), Supervisor of more than ten master- and bachelor theses.

10.2007-9.2010 **Fraunhofer Institute for Mechanics of Materials IWM**

Wöhlerstrasse 11, 79 108 Freiburg im Breisgau, Germany

Ab-initio calculations and atomistic simulations of defect-related properties in ferroelectric oxides, lead-free ferroelectrics, multiscale modelling of ferroelectric materials

2004-2007 **Institute of Physics ASCR and Charles University**

Doctoral thesis: Simulation of domain structure formation in ferroelectric materials

Development of the computer code **ferrodo**

2001-2003 **Institute of Physics ASCR and Czech Technical University**

Master thesis: Selection rules for inelastic neutron scattering

Publication record

44 publications in impacted journals (10 within the last 5 years), 1070 citations, h-index: 17 (SCOPUS)

Scientific interests

- Expert in the field of **ferroelectric materials**: ferroic domains and domain walls, phase transitions, phenomenological phase-field-type modelling, Landau theory, development of model parametrizations for simulations.
- Expert in **ab-initio** and **classical modelling of ferroelectrics**.
- Author of a large simulation package **ferrodo for simulation of development of ferroelectric domain structure** under various external influences.
- Expert in **programming** (C/C++, Python, Linux shell, Perl),
- Expert in **vibration damping** using the active-elasticity control approach.

International conferences

More than 50 contributions (more than 40 talks including 3 invited). Invited contributions:
- Joint IEEE ISAF-IWATMD-PFM Conference, Atlanta 2017
- The International Meeting on Ferroelectricity, San Antonio 2017
- Polish-Czech Seminar on Structural and Ferroelectric Phase Transitions, Kouty 2018

Research interests and recent activity

Phenomenological modelling of ferroelectric domains and domain walls. Development and maintenance of the **simulation package ferrodo** (of which I am a principal author), designed for modelling of formation and evolution of domain structures in ferroelectric materials. First-principles and atomistic shell-model simulations of static and dynamical processes in solids. Bridging scales between models of solids. Nuclear magnetic resonance. Suppression of vibration damping using active-elasticity control. **The main works related to the project are**: (i) parametrization of the Landau-Devonshire model for $BiFeO_3$ using first-principles calculatiosn [**Phys. Rev. B 96, 174110 (2017)**]; the same methodology was recently successfully used for other perovskites as well (ii) ab-initio calculations and atomic-level simulations in multiferroic $BiFeO_3$ showing substantial enhancement of its permittivity in the domain walls [**Phys. Rev. Lett. 119, 057604 (2017)**], (iii) analysis of discretization-related effects in phase-field modelling of domain walls [**Phase Transitions 91, 959 (2018)**], (iv) detailed investigation of Ising lines appearing within Bloch-type domain walls in $BaTiO_3$ [**Phys. Rev. B 92, 094106 (2015)**] and study of structure of ferroelectric nanoparticles [**Phys Rev. B 89, 060101 (2014)**], (v) Simulations domains in metal-ferroelectric super-crystals [**Nature Materials 20, 495 (2021)**].

Teaching

Courses on Quantum mechanics, Physics of solid-state materials and Electricity, magnetism and optics

Supervision of more than fifteen master- and bachelor- theses

Supervision of 1 doctoral student of the nanotechnological study branch (defended in 2018)

Serving scientific community

Organizing activities

ABINIT school on ground state and linear response properties, Prague, Czech Republic, 2–6 September 2019

Grant reviewer

Deutsche Forschungsgemeinschaft (DFG)
Israel Science Foundation (ISF)
National Natural Science Foundation of China (NSFC)

Journal reviewer

Physical Review Letters (APS), Physical Review B (APS), Physical Review Applied (APS), npj Quantum Materials (Nature), Acta Materialia (Elsevier), Journal of Applied

Physics (AIP Publishing), Ferroelectrics (Taylor & Francis), Phase Transitions (Taylor & Francis), Europhysics Letters (European Physical Society), Computational Materials Science (Elsevier)

Participation in grants

2004-2007 **GAČR 202/05/H003**: Physics of complex physical systems (member of the team)
2006-2007 **GAČR 202/06/0411**: Domain phenomena in ferroic materials (member of the team)
2007-2010 **German Federal Ministry of Education and Research (BMBF) Framework Programme WING, Project Code 03X0510**: Computer-based multiscale modelling for design of polycrystalline ferroelectric materials for actuators and sensors (COMFEM) (member of the team)
2010-2012 **GAČR P204/10/0616**: Modern piezoelectric perovskites: Lattice vibrations and domain walls (member of the team)
2010-2013 **MPO FR-TI2/165**: Piezoelectric ceramics of new generation (member of the team)
2013-2015 **GAČR 13-10365S**: Planar acoustic metamaterials with the active control of acoustic impedance (member of the team)
2015-2017 **GAČR 15-04121S**: Emergent perspectives of ferroelectric interfaces (member of the team)
2017-2019 **GAČR 17-11494J**: Multiferroicity in skyrminonic materials (member of the team)
2018-2022 Operational Programme Research, Development and Education financed by European Structural and Investment Funds and the Czech Ministry of Education, Youth and Sports: SOLID21 – CZ.02.1.01/0.0/0.0/16_019/0000760 (member of the team)
2021-2023 **GAČR 21-20110K**: Semiconductor – dielectric heterostructures for photoelectrochemical hydrogen evolution (SeDiHe) (member of the team)
2021-2025 **H2020-EU.1.2.1. - FET Open**: Topological Solitons in Antiferroics (TSAR) (member of the team)

Complete bibliography

1. Metal-ferroelectric supercrystals with periodically curved metallic layers, Hadjimichael, M. and Li, Y. and Zatterin, E. and Chahine, G.A. and Conroy, M. and Moore, K. and O'Connell, E.N. and Ondrejkovic, P. and Marton, P. and Hlinka, J. and Bangert, U. and Leake, S. and Zubko, P., Nature Materials, 2021, 20(4), pp. 495–502
2. Anisotropic Strain in Rare-Earth Substituted Ceria Thin Films Probed by Polarized Raman Spectroscopy and First-Principles Calculations, Sediva, E., Bohdanov, D., Harrington, G.F., ...Marton, P., Hlinka, J., ACS Applied Materials and Interfaces, 2020, 12(50), pp. 56251–56259
3. Discretisation originated Peierls–Nabarro barriers in simulations of ferroelectrics, Marton, P., Phase Transitions, 2018, 91(9-10), pp. 959–968
4. Far-infrared reflectivity spectra of nanotwinned GaV4Se8, Dočekalová, Z., Marton, P., Ondrejkovic, P., Hlinka, J., Phase Transitions, 2018, 91(9-10), pp. 942–952
5. The elastic properties of an actively controlled piezoelectric transducer: Measurement, analysis and tuning, Marton, P., Nečásek, J., Václavík, J., Mokrý, P., Journal of Sound and Vibration, 2018, 415, pp. 78–90
6. Construction of wide tuneable volume radiofrekvency coil for mr imaging of small rodents | Konstrukce široce přeladitelné objemové radiofrekvenční cívky pro mr zobrazování malých hlodavců, Vít, M., Marton, P., Burian, M., Gálisová, A., Jirák, D., Ceska Radiologie, 2018, 72(3), pp. 196–203
7. First-principles-based Landau-Devonshire potential for BiFeO3, Marton, P., Klíč, A., Paściak, M., Hlinka, J., Physical Review B, 2017, 96(17), 174110
8. Terahertz-Range Polar Modes in Domain-Engineered BiFeO3, Hlinka, J., Paściak, M., Körbel, S., Marton, P., Physical Review Letters, 2017, 119(5), 057604

9. Comparison of analog front-ends for digital synthetic impedance device, Necasek, J., Vaclavik, J., Marton, P., Proceedings of the 2017 IEEE International Workshop of Electronics, Control, Measurement, Signals and their Application to Mechatronics, ECMSM 2017, 2017, 7945916
10. Digital synthetic impedance for application in vibration damping, Nečásek, J., Václavík, J., Marton, P., Review of Scientific Instruments, 2016, 87(2), 024704
11. Ferroelectric domain walls and their intersections in phase-field simulations, Hlinka, J., Stepkova, V., Marton, P., Ondrejkovic, P., Springer Series in Materials Science, 2016, 228, pp. 161–180
12. Ising lines: Natural topological defects within ferroelectric Bloch walls, Stepkova, V., Marton, P., Hlinka, J., Physical Review B - Condensed Matter and Materials Physics, 2015, 92(9), 094106
13. Fast and portable precision impedance analyzer for application in vibration damping, Nečásek, J., Václavík, J., Marton, P., Proceedings of the 2015 IEEE International Workshop of Electronics, Control, Measurement, Signals and their Application to Mechatronics, ECMSM 2015, 2015, 7208693
14. Lattice dynamics of NaI studied by inelastic neutron scattering: Absence of thermally induced discrete breathers, Kempa, M., Ondrejkovic, P., Bourges, P., Marton, P., Hlinka, J., Physical Review B - Condensed Matter and Materials Physics, 2014, 89(5), 054308
15. Closed-circuit domain quadruplets in BaTiO 3 nanorods embedded in a SrTiO 3 film, Stepkova, V., Marton, P., Setter, N., Hlinka, J., Physical Review B - Condensed Matter and Materials Physics, 2014, 89(6), 060101
16. Peculiar domain states of cylindrical BaTiO3 nanorods embedded in SrTiO3 matrix, Stepkova, V., Marton, P., Hlinka, J., Phase Transitions, 2014, 87(10-11), pp. 922–928
17. Noise shielding using active acoustic metamaterials with electronically tunable acoustic impedance, Mokrý, P., Steiger, K., Václavík, J., ...Kodejška, M., Černík, M., INTERNOISE 2014 - 43rd International Congress on Noise Control Engineering: Improving the World Through Noise Control, 2014
18. Influence of the A/b stoichiometry on defect structure, sintering, and microstructure in undoped and Cu-doped KNN, Hoffmann, M.J., Kungl, H., Acker, J., ...Erünal, E., Jakes, P., Lead-Free Piezoelectrics, 2013, 9781441995988, pp. 209–251
19. Piezoelectric properties of twinned ferroelectric perovskites with head-to-head and tail-to-tail domain walls, Ondrejkovic, P., Marton, P., Guennou, M., Setter, N., Hlinka, J., Physical Review B - Condensed Matter and Materials Physics, 2013, 88(2), 024114
20. Phonon frequencies of tetragonally strained PbTiO3 from first principles, Marton, P., Hlinka, J., Phase Transitions, 2013, 86(2-3), pp. 200–205
21. Design of wall-plug efficiency optimized semi-active Piezoelectric Shunt Damping systems, Václavík, J., Mokrý, P., Márton, P., 2013 Joint IEEE International Symposium on Applications of Ferroelectric and Workshop on Piezoresponse Force Microscopy, ISAF/PFM 2013, 2013, pp. 325–328, 6748748
22. Divergence of dielectric permittivity near Phase transition within ferroelectric domain boundaries, Marton, P., Stepkova, V., Hlinka, J., Phase Transitions, 2013, 86(1), pp. 103–108
23. Planar acoustic metamaterials with the active control of acoustic impedance using a piezoelectric composite actuator, Nováková, K., Psota, P., Doleček, R., ...Márton, P., Černík, M., 2013 Joint IEEE International Symposium on Applications of Ferroelectric and Workshop on Piezoresponse Force Microscopy, ISAF/PFM 2013, 2013, pp. 317–320, 6748720
24. Bloch-type domain walls in rhombohedral BaTiO 3, Taherinejad, M., Vanderbilt, D., Marton, P., Stepkova, V., Hlinka, J., Physical Review B - Condensed Matter and Materials Physics, 2012, 86(15), 155138
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26. Stress-induced phase transition in ferroelectric domain walls of BaTiO 3, Stepkova, V., Marton, P., Hlinka, J., Journal of Physics Condensed Matter, 2012, 24(21), 212201

27. First-principles study of structural and elastic properties of the tetragonal ferroelectric perovskite Pb(Zr0.50Ti0.50)O3, Marton, P., Elsässer, C., Physica Status Solidi (B) Basic Research, 2011, 248(10), pp. 2222–2228
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29. Phase-field modelling of 180° bloch walls in rhombohedral BaTiO3, Hlinka, J., Stepkova, V., Marton, P., ...Janovec, V., Ondrejkovic, P., Phase Transitions, 2011, 84(9-10), pp. 738–746
30. Coexistence of rectilinear and vortex polarizations at twist boundaries in ferroelectric PbTiO3 from first principles, Shimada, T., Wang, X., Tomoda, S., ...Elsässer, C., Kitamura, T., Physical Review B - Condensed Matter and Materials Physics, 2011, 83(9), 094121
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33. Formation of vacancies and copper substitutionals in potassium sodium niobate under various processing conditions, Körbel, S., Marton, P., Elsässer, C., Physical Review B - Condensed Matter and Materials Physics, 2010, 81(17), 174115
34. Domain walls of ferroelectric BaTiO3 within the Ginzburg-Landau-Devonshire phenomenological model, Marton, P., Rychetsky, I., Hlinka, J., Physical Review B - Condensed Matter and Materials Physics, 2010, 81(14), 144125
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36. The piezoelectric response of nanotwinned BaTiO3, Hlinka, J., Ondrejkovic, P., Marton, P., Nanotechnology, 2009, 20(10), 105709
37. Ferroelastic domain walls in barium titanate-quantitative phenomenological model, Hlinka, J., Marton, P., Integrated Ferroelectrics, 2008, 101(1), pp. 50–62
38. Computer simulations of frequency-dependent dielectric response of 90-degree domain walls in tetragonal barium titanate, Marton, P., Hlinka, J., Ferroelectrics, 2008, 373(1 PART 1), pp. 139–144
39. Phenomenological model of a 90° domain wall in BaTi O3 -type ferroelectrics, Hlinka, J., Márton, P., Physical Review B - Condensed Matter and Materials Physics, 2006, 74(10), 104104
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