andrius.merkys@
gmail.com
+370 613 12191

Address
Saulėtekio al. 7–C521
LT-10257 Vilnius
Lithuania

Andrius Merkys

Researcher

About Me Researcher, scientific software developer and server manager with 12 years of experience. Participated in national and multinational European scientific projects, including the development of Crystallography Open Database and AiiDA. Proficient in cheminformatics, crystallography, data analysis, statistics, server administration, Web technologies and both low- and high-level programming languages. Experienced in working with large multinational teams with both direct and written communication. Skilled in organization and presentation.

Education

2007 – 2011, Vilnius University
BSc in Bioinformatics

2011 – 2013, Vilnius University
MSc in Computer Science

2013 – 2018, Vilnius University
PhD in Chemistry Engineering

Experience

Jul 2010 – present, *Researcher*, Vilnius University
Development of the Crystallography Open Database in Vilnius University Institute of Biotechnology, Department of Protein–DNA Interactions

Jun 2012 – Jul 2012, *Research Support*,
Laboratory of Molecular Biology
Research in UK Medical Research Council's Laboratory of Molecular Biology, Department of Structural Studies

Oct 2014 – Oct 2015, *Doctoral Assistant*,
École Polytechnique Fédérale de Lausanne
Development of AiiDA framework in École Polytechnique Fédérale de Lausanne, Laboratory of Theory and Simulation of Materials THEOS

Since Mar 2019, *Debian Developer*, Debian
Voluntary contributions to scientific packages in Debian

Since May 2019, *Advisory Board Member*,
Crystallography Open Database
Member of the international advisory committee for the development of the Crystallography Open Database

Communication Skills

Since 2013, 10+ poster presentations in scientific conferences
Presented my research in conferences worldwide.

Since 2017, 5 courses for BSc and MSc students
Prepared and read Bioinformatics courses in Vilnius University.

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Publications

OPTIMADE, an API for exchanging materials data
Andersen et al. (2021). Scientific Data, 8,
https://doi.org/10.1038/s41597-021-00974-z

Validation of the Crystallography Open Database using the Crystallographic Information Framework
Vaitkus et al. (2021). Journal of Applied Crystallography, 54,
https://doi.org/10.1107/S1600576720016532

AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance
Huber et al. (2020). Scientific Data, 7,
https://doi.org/10.1038/s41597-020-00638-4

Raman Open Database: first interconnected Raman–X-ray diffraction open-access resource for material identification
El Mendili et al. (2019). Journal of Applied Crystallography, 52,
https://doi.org/10.1107/S1600576719004229

Using SMILES strings for the description of chemical connectivity in the Crystallography Open Database
Quirós et al. (2018). Journal of Cheminformatics, 10, 1
https://doi.org/10.1186/s13321-018-0279-6

Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds
Mounet et al. (2018). Nature Nanotechnology, 13, 3
https://doi.org/10.1038/s41565-017-0035-5

A posteriori metadata from automated provenance tracking: integration of AiiDA and TCOD
Merkys et al. (2017). Journal of Cheminformatics, 9, 1
https://doi.org/10.1186/s13321-017-0242-y

AceDRG: a stereochemical description generator for ligands
Long et al. (2017). Acta Crystallographica Section D
https://doi.org/10.1107/s2059798317000067

Validation and extraction of molecular-geometry information from small-molecule databases
Long et al. (2017). Acta Crystallographica Section D
https://doi.org/10.1107/s2059798317000079

COD::CIF::Parser: an error-correcting CIF parser for the Perl language
Merkys et al. (2016). Journal of Applied Crystallography, 49,
https://doi.org/10.1107/s1600576715022396

Computing stoichiometric molecular composition from crystal structures
Gražulis et al. (2015). Journal of Applied Crystallography, 48,
https://doi.org/10.1107/s1600576714025904

Crystallography Open Database (COD): an open-access collection of crystal structures and platform for world-wide collaboration
Gražulis et al. (2012). Nucleic Acids Research, 40, D1
https://doi.org/10.1093/nar/gkr900

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Projects

Chemical annotation in the Crystallography Open Database (COD)
Research Council of Lithuania, 2020-03-01 – 2022-12-31,
principal investigator – Andrius Merkys

Sonic drilling coupled with automated mineralogy & chemistry
European Union's Horizon 2020 research and innovation program,
2016-02-01 – 2020-08-31

CODEX – Computational and crystallographic open data exchange
Scientific Exchange Programme between the New Member States of the EU and Switzerland, 2014-10-01 – 2015-10-31,
principal investigator – Andrius Merkys

Expansion for the Crystallography Open Database (COD) and statistical analysis of crystal structures
Research Council of Lithuania, 2013-03-01 – 2015-09-30,
principal investigator – Saulius Gražulis

Open access crystallographic database COD
Research Council of Lithuania, 2010 – 2011,
principal investigator – Saulius Gražulis

Awards

PRACE HPC Excellence Award 2022 (with co-authors)
For work on *Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds*, as described in publication in Nature Nanotechnology 13, 246–252 (2018)

ACCES Visualization Contest 2015
First Prize in the Image category

Software Development Skills

Programming

- C
- Perl
- Python
- Bash
- Go
- PHP

Computer Software

- Apache2
- Debian/Linux
- MariaDB/MySQL