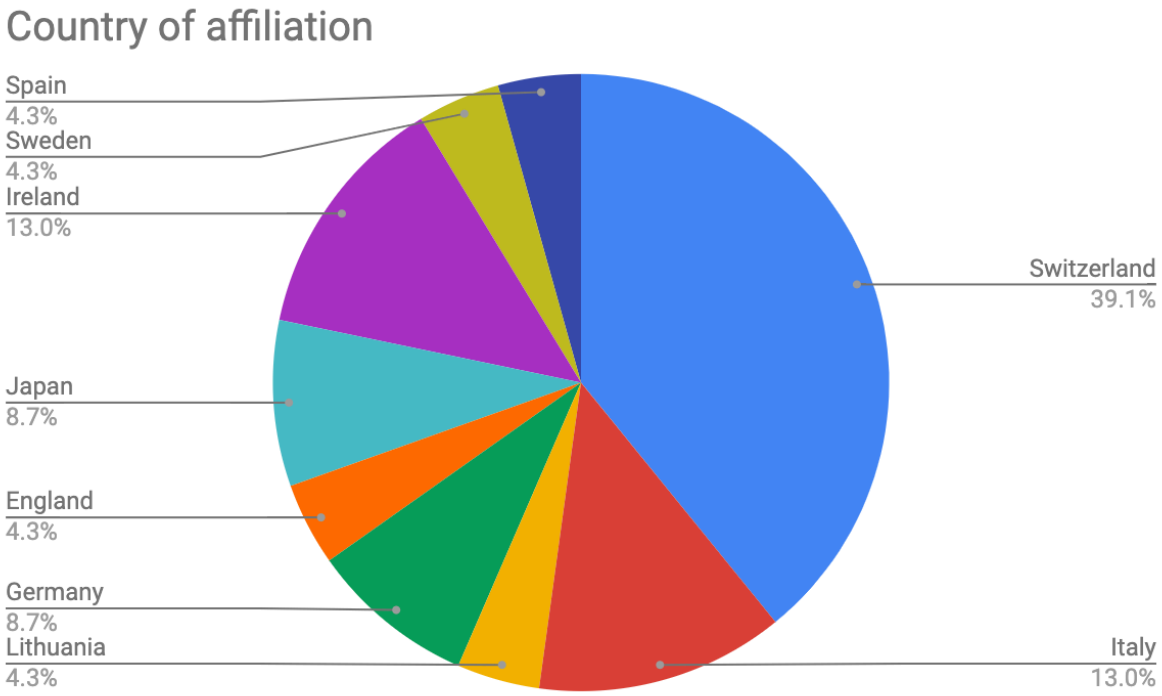
AiiDA-powered research projects

- Questionnaire on AiiDA mailing list
  - 27 research projects
  - 25 plugins



Project status: published

Project title	DOI
Two-dimensional materials from high-throughput computational exfoliation of experimentally known compounds [1]	10.1038/s41565-017-0035-5
Arsenene MOSFET [2]	10.1038/ncomms12585
Polar discontinuities [3]	10.1038/ncomms6157
Ideal adhesive and shear strengths of solid interfaces: A high throughput ab initio approach [4]	10.1016/j.commatsci.2018.08.006
Storing reproducible workflows in the Theoretical Crystallography Open Database [5]	10.1186/s13321-017-0242-y
Ab-initio studies for battery materials design [6]	10.1103/PhysRevMaterials.2.103805
SSSP Pseudopotential libraries [7]	10.1038/s41524-018-0127-2
Electronic and optical properties of doped TiO_2 by many-body perturbation theory [8]	10.1103/PhysRevMaterials.3.045401

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[1] N. Mounet et al., Nat. Nanotech. 13, 246 (2018)
[2] G. Pizzi et al., Nat Comm. 7, 12585 (2016)
[3] M. Gibertini et al., Nat. Comm. 5, 5157 (2014)
[4] P. Restuccia et al., Comp. Mat. Sci. 154, 517 (2018)
[5] A. Merkys et al., J. Cheminf. 9, 56 (2017)
[6] D. Gresch et al., Phys. Rev. Materials 2, 103805 (2018)
[7] G. Prandini et al., npj Comp. Mat. 4, 72 (2018)
[8] M. O. Atambo et al., Phys. Rev. Mat. 3, 045401 (2019)

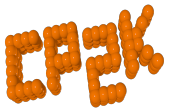
Project status: simulations completed

Project title	Email
A high-throughput search for new solid-state electrolytes for Li-ion batteries	leonid.kahle@epfl.ch
Applicability of tail-corrections in the molecular simulations of porous materials	kevin.jablonka@epfl.ch
Determining interface structures between fluorite and pervoskite materials	bz240@cam.ac.uk
Lattice thermal conductivities of materials	fyuewen@gmail.com
Siesta LDA pseudo test	bosonie@tcd.ie
Gas adsorption in covalent organic frameworks	daniele.ongari@epfl.ch
Ab-initio studies for battery materials design	andreas.stamminger@de.bosch.com

AiiDA plugins

raspa2 zeo++

phonopy



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Project status: underway

Project title	Email
Transferability of Machine Learning Models for Complex Properties of Porous Materials	kevin.jablonka@epfl.ch
Systematic study of the Atomic Self Interaction Correction	bosonie@tcd.ie
High-Throughput simulations of Complex Band Structures	bosonie@tcd.ie
3DD	sebastiaan.huber@epfl.ch
High-throughput Investigation of the Effect of Impurities on the Transport Properties of Topological Insulators	p.ruessmann@fz-juelich.de
Graphene adhesion on surfaces: a van der Waals density functional study	elgammal@kth.se
Simulation of Water Isotherms	kevin.jablonka@epfl.ch
Flat-land nanoelectronics	vm.garcia@cinn.es
High throughput phonon calculation	togo.atsushi@gmail.com
GW convergence workflows	miki.bonacci@unimore.it

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