Geoffroy Hautier

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Professional Experience

2018-now **Dartmouth College**, *Associate Professor*, Thayer School of Engineering.

2018-now **Université catholique de Louvain**, *Associate Professor*, Institute of Condensed Matter and Nanoscience, School of Chemistry.

2014-2018 **Université catholique de Louvain**, *Assistant Professor*, Institute of Condensed Matter and Nanoscience, School of Chemistry.

2011-2014 **FNRS**, *postdoctoral researcher*, work carried on at the Université catholique de Louvain with Prof. Xavier Gonze.

2011 **Massachusetts Institute of Technology**, *postdoctoral researcher*.

2006–2011 **Massachusetts Institute of Technology**, *research assistant*.

2004–2006 **FWO**, *aspirant*, work carried on at Katholieke Universiteit Leuven (KUL) and IMEC.

Education

2006–2011 **Massachusetts Institute of Technology**, *PhD in Materials Science and Engineering*. High-Throughput Data Mined Prediction of Inorganic Compounds and Computational Discovery of New Lithium-Ion Battery Cathode Materials. Advisor: Professor Gerbrand Ceder.

1999–2004 **Université Libre de Bruxelles**, *Materials Science and Engineering degree*, Ingénieur civil en Science des Matériaux.

2001–2004 **Ecole Centrale Paris**, *Engineering degree*, Ingénieur centralien, TIME double-degree program.

Organization of workshops and conference symposia

March 2021 **American Physical Society (APS) meeting**, *co-organizer of a symposium on Computational Design and Discovery of Novel Materials*, Nashville, TN, USA.

September 2019 **European-Materials Research Society (E-MRS), Fall**, *co-organizer of a symposium on Fabrication and characterization of emerging transparent conductive materials*, Warsaw, Poland.

July 2019 **47th IUPAC World Chemistry Congress**, *co-organizer of a symposium on Materials for Energy by Computational Design*, Paris, France.

May 2019 **European-Materials Research Society (E-MRS), Spring**, *co-organizer of a symposium on Earth-abundant next generation materials for solar energy*, Nice, France.

May 2017 **European-Materials Research Society (E-MRS), Spring**, *lead organizer of a symposium on earth abundant and emerging solar energy conversion materials*, Strasbourg, France.

October 2016 **Lorentz Workshop**, *co-organizer of a Lorentz workshop on Open Databases Integration for Materials Design* , Leiden, Netherlands.

May 2016 **Materials Research Society (MRS), Spring**, *co-organizer symposium on Materials, Interfaces and Devices by Design*, Phoenix, USA.

May 2015 **European-Materials Research Society (E-MRS), Spring**, *co-organizer symposium on earth abundant and emerging solar energy conversion materials*, Lille, France.

Supervision of students and participation to thesis committees

September 2014-Present **Supervision of PhD students**, *Université catholique de Louvain*, Louvain-La-Neuve, Belgique.

- Romain Claes, PhD in Science, 2019-
- Volodia Gounaris, PhD in Science, 2018-
- Diana Daliah, PhD in Applied Sciences and Engineering, 2018-
- Yasmine Benabed, PhD in Science, joint PhD with Montréal University, 2018-
- Guillaume Brunin, PhD in Applied Sciences and Engineering, 2016-
- Jan Kloppenburg, PhD in Science, 2015-
- Viet Anh Ha, PhD in Applied Sciences and Engineering, 2014-2018
- Gil Vander Marcken, PhD in Science, 2014-2018

September 2014-Present **Supervision of Master thesis students**, *Université Catholique de Louvain*, Louvain-La-Neuve, Belgique.

- Louis Alaerts, student in Chemistry, 2018
- Gabriel Closset, student in Chemistry, 2018
- Romain Claes, student in Chemistry, 2018
- Volodia Gounaris, student in Chemistry, 2018
- Louis Storm, student in Applied Physics, 2017
- Grégoire Thunis, student in Applied Physics, 2016
- Jean-Baptiste Van den Eyde, student in Applied Physics, 2016
- Guillaume Brunin, student in Applied Physics, 2016
- Emile Fourneau, student in Materials Science and Engineering, 2015

September 2014-Present **PhD thesis committees**.

- Leonid Kahle, PhD at Ecole Polytechnique Fédérale de Lausanne (EPFL), planned graduation in 2019
- Francesco Naccarato, PhD at UCLouvain and Luxemburg University, 2019
- Nicolas Dardenne, PhD at UCLouvain, 2019
- Korina Kuhar, PhD at Denmark Technical University (DTU), 2017
- Sriram Poyyapakkam Ramkumar, PhD at UCLouvain, 2017
- Natalia Tumanova, PhD at UCLouvain, 2017
- Yohandys Zulueta, PhD at KULeuven, 2017

September 2013 **Reader and member of a jury for Engineering master thesis**, *Université Catholique de Louvain*, Louvain-La-Neuve, Belgique.

- Read and grade a master thesis
- Member of the jury grading the students' presentations

October 2011-Present **Member of the jury for the Photovoltaic (P3) Project**, *Université Catholique de Louvain*, Louvain-La-Neuve, Belgique.

- Read and grade students' final report
- Member of the jury grading the students' presentations and reports

Teaching

2019- **Physical Chemistry II, 1st year master in chemistry**, *Université Catholique de Louvain*, Louvain-La-Neuve, Belgique.

2014- **Quantum chemistry, 3d year bachelor in chemistry**, *Université Catholique de Louvain*, Louvain-La-Neuve, Belgique.

2014- **Elements of Molecular Physical Chemistry, 2d year bachelor in chemistry**, *Université Catholique de Louvain*, Louvain-La-Neuve, Belgique.

2015- **General Chemistry, 2d year bachelor in chemistry and bioengineering**, *Université Catholique de Louvain*, Louvain-La-Neuve, Belgique.

Service to the University

2019- **Member of the FRIA jury**, Brussels, Belgium.

- Member of the commission attributing FRIA PhD fellowships

2019- **Representative of the Institute of Condensed Matter and Nanosciences at UCLouvain Center for High Performance Computing and Mass Storage (CISM)**, Louvain-la-Neuve, Belgium.

2019 **Member of the jury for the Belgian American Education Foundation Fellowship**, Brussels, Belgium.

- Member of the jury attributing the fellowship

2015 **Working group on a materials chemistry class**, *Université Catholique de Louvain*, Louvain-La-Neuve, Belgium.

- Member of the working group developing a new class in materials chemistry

2015-2018 **Teaching assistant commission**, *Université Catholique de Louvain*, Louvain-La-Neuve, Belgium.

- Member of the commission attributing teaching assistant positions for the Faculty of Science, school of chemistry

Awards and Fellowships

2019 **Chemistry of Materials Reviewer Excellence Award**.

2018 **Finalist of the Rising Star in Computational Materials Science Prize for 2018**, *prize organized by the journal Computational Materials Science.*

2018 **Chemistry of Materials Reviewer Excellence Award**.

2016 **Invited paper in Chemistry of Materials**, *special edition on "Computational Design of Functional Materials".*

2016 **Emerging investigator for Journal of Materials Chemistry C**, *invited paper in a special edition.*

Oct. 2011–Sept. 2014 **FNRS-FRS Chargé de Recherche**, *postdoctoral fellowship*, proposal graded "A - very good to excellent".

2011 **Incoming post-doctoral Fellowships co-funded by the Marie Curie Actions of the European Commission**, *2 year postdoctoral fellowship awarded but declined in favor of the FNRS fellowship*, proposal graded 93/100 (among the 2% best).

September 2008–June 2009 **TOTAL-MIT Energy Fellowship**.

September 2006–June 2007 **Belgian American Education Foundation (BAEF) Fellowship**.

September 2004–June 2006 **Fonds voor Wetenschappelijk Onderzoek (FWO) Fellowship**.

2004 **Medal of Université Libre de Bruxelles**, *award delivered on graduation to the ULB students with the most prestigious academic record.*

Selected interviews and articles in the general and specialized press

February 2020 **Chemistry World**, *February 24 2020*, Textbook structure rules formulated by Linus Pauling 90 years ago prove unreliable, article about my Angewandte paper about the Pauling rules.
http://www.chemistryworld.com/news/textbook-structure-rules-formulated-by-linus-pauling-90-years-ago-prove-unreliable/4011236.article

September 2019 **MRS Bulletin News**, *September 26 2019*, Electride with partially filled d-subshell discovered, article about my JACS paper on electrides.
http://www.cambridge.org/core/journals/mrs-bulletin/news/electride-with-partially-filled-d-subshell-discovered

July 2019 **Naked Scientist**, *August 14 2019*, Less flammable batteries?, article about my work on Li-ion batteries in a major scientific blog.
http://www.thenakedscientists.com/articles/science-news/less-flammable-batteries

July 2019 **RTBF daily news**, *July 18 2019*, interview about my research in Li-ion batteries in the daily news for the main public Belgian TV channel.
http://www.rtbf.be/auvio/detail_innovation-la-batterie-du-futur?id=2522635

July 2019 **RTL-TVI daily news**, *July 17 2019*, interview about my research in Li-ion battery in the daily news for the main private Belgian TV channel.
http://www.rtl.be/info/video/714418.aspx?fbclid=IwAR1rmmLVe-UURgzXermDlgOTiJvua-aOMrm-L3hpEDxxoulgcnaHrqAU6Ho

July 2019 **L'écho**, *July 17 2019*, Des chercheurs de l'UCLouvain découvrent un matériau clé pour la batterie du futur, article in the most read economical Belgian newspaper on my work on Li-ion battery.
http://www.lecho.be/entreprises/energie/des-chercheurs-de-l-uclouvain-decouvrent-un-materiau-cle-pour-la-batterie-du-futur/10145890.html

July 2019 **Le Soir**, *July 17 2019*, L'UCLouvain découvre le matériau de la batterie du futur, article in a major Belgian newspaper on my work on Li-ion batteries.
http://plus.lesoir.be/237115/article/2019-07-17/luclouvain-decouvre-le-materiau-de-la-batterie-du-futur

September 2016 **Le Soir**, *September 21 2016*, La céramique, c'est chic, article in a major Belgian newspaper for which I was interviewed as an expert in Materials Science.
http://plus.lesoir.be/60377/article/2016-09-21/la-ceramique-cest-chic

June 2015 **Chemical and Engineering News**, *June 10 2015*, Searching The Periodic Table For Novel Solids, comment on a paper for which I was interviewed as an expert in computational materials science.
https://cen.acs.org/articles/93/web/2015/06/Searching-Periodic-Table-Novel-Solids.html

February 2014 **MIT news**, *February 4 2014*, Materials database proves its mettle with new discoveries, article on high-throughput computing and the Materials Project in which I was interviewed.
http://newsoffice.mit.edu/2014/materials-database-proves-its-mettle-with-new-discoveries-0204

June 2014 **FNRS news**, *June 2014 p. 30-31*, Les ordinateurs, une aide précieuse pour les scientifiques, article in the magazine of the national science foundation in Belgium on my research on transparent conducting oxides.
http://www.frs-fnrs.be/docs/Lettre/lettre97.pdf

January 2013 **La Libre Belgique**, *28 January 2013, p.15*, Le casse-tête des métaux rares, article on my research on transparent conducting oxides in one of the major Belgian newspaper.

July 2012 **L'usine Nouvelle**, *3294-3295, 12 July 2012 , p. 80-81* , Conception : Les matériaux au crible de l'ordinateur, article on high-throughput computing in which I was interviewed in a technology/business French magazine.
http://www.usinenouvelle.com/article/conception-les-materiaux-au-crible-de-l-ordinateur.N178593

Peer-Reviewing, Editorial and Scientific Society Activities

Associate editor for npj computational materials

Editorial board member for iScience

Group leader for the working group high-throughput screening and data analyticd from the psi-k society

Frequent **reviewer** for Nature Materials, Nature Communications, Energy and Environmental Sciences, Advanced Materials, Journal of the American Chemical Society, Chemistry of Materials, Joule, Chem, Physical Review B, Physical Review Materials, and Physical Review X

Reviewer for proposals submitted to the US Department of Energy (DOE)-Basic Energy Sciences (BES), the ACS Petroleum Research Fund, the French National Research Agency, the German research agency (Deutsche Forschungsgemeinschaft, DFG), the Swiss National Science Foundation (SNF) and the Israel Science Foundation (ISF)

Bibliometric indicators

h-factor: 43

citations: 12 626

according to google scholar: http://scholar.google.com/citations?user=eDZ_BlkAAAAJ&hl=en

Book chapters

1 **G. Hautier**, *Data mining approaches to high-throughput crystal structure and compound prediction*, book chapter for the serie: Topics in Current Chemistry, Prediction and Calculation of Crystal Structures: Methods and Applications, 2013

Publications (Peer-reviewed)

1 V.-A. Ha, B. Karasulu, R. Maezono, G. Brunin, J. B. Varley, G.-M. Rignanese, B. Monserrat, **G. Hautier** *Boron phosphide as a -type transparent conductor: Optical absorption and transport through electron-phonon coupling*, Physical Review Materials, 4, 065401, 2020

2 I. T. Witting, F. Ricci, T. C. Chasapis, **G. Hautier**, G. J. Snyder *The Thermoelectric Properties of-Type Bismuth Telluride: Bismuth Selenide Alloys*, Research, 2020, 4361703, 2020

3 A. Champagne, F. Ricci, M. Barbier, T. Ouisse, D. Magnin, S. Ryelandt, T. Pardoen, **G. Hautier**, M.W. Barsoum, J.-C. Charlier *Insights into the elastic properties of RE-i-MAX phases and their potential exfoliation into two-dimensional RE-i-MXenes*, Physical Review Materials, 4, 013604, 2020

4 J. George, D. Waroquiers, D. Di Stefano, G. Petretto, G. Rignanese, **G. Hautier** *The limited predictive power of the pauling rules*, Angewandte Chemie, 132, 7639, 2020

5 Z. Ma, A. Jaworski, J. George, A. Rokicinska,T. Thersleff, T. Budnyak, G. Hautier, A. J. Pell, R. Dronskowski, P. Kuśtrowski, A. Slabon *Exploring the Origins of Improved Photocurrent by Acidic Treatment for Quaternary Tantalum-Based Oxynitride Photoanodes on the Example of CaTaO2N*, J. Phys. Chem. C, 124, 152, 2019

6 X. Gonze, B. Amadon, G. Antonius, F. Arnardi, L. Baguet, J.-M. Beuken, J. Bieder, F. Bottin, J. Bouchet, E. Bousquet, N. Brouwer, F. Bruneval, G. Brunin, T. Cavignac, J.-B. Charraud, W. Chen, M. Côté, S. Cottenier, J. Denier, G. Geneste, P. Ghosez, M. Giantomassi, Y. Gillet, O. Gingras, D. R. Hamann, **G. Hautier**, X. He, N. Helbig, N. Holzwarth, Y. Jia, F. Jollet, W. Lafargue-Dit-Hauret, K. Lejaeghere, M. AL Marques, A. Martin, C. Martins, H. PC Miranda, F. Naccarato, K. Persson, G. Petretto, V. Planes, Y. Pouillon, S. Prokhorenko, F. Ricci, G.-M. Rignanese, A. H Romero, Mi. Marcus Schmitt, M. Torrent, M. J van Setten, B. Van Troeye, M. J Verstraete, G. Zérah, J. W Zwanziger, *The Abinit project: Impact, environment and recent developments*, Computer Physics Communications, 107042, 2019

7 S. Hadke, W. Chen, J. M. Rui Tan, M. Guc, V. Izquierdo-Roca, G.-M. Rignanese, **G. Hautier**, L. H. Wong, *Effect of Cd on cation redistribution and order- disorder transition in Cu2(Zn,Cd)SnS4*, Journal of Materials Chemistry A, 7, 26927, 2019

8 P. Chanhom, K. E. Fritz, L. A. Burton, J. Kloppenburg, Y. Filinchuk, A. Senyshyn, M. Wang, Z. Feng, N. Insin, J. Suntivich, **G. Hautier**, *Sr3CrN3: A New Electride with a Partially Filled d- Shell Transition Metal*, Journal of the American Chemical Society, 141, 10595-10598, 2019

9 D. Di Stefano, A. Miglio, K. Robeyns, Y. Filinchuk, M. Lechartier, A. Senyshyn, H. Ishida, S. Spannenberger, M. Wilkening, B. Roling Y. Katoh and **G. Hautier**, *Superionic diffusion through frustrated energy landscape*, Chem, 5, 2450, 2019

10 W. Chen, J. George, J. B. Varley, G.-M. Rignanese, and **G. Hautier**, *High-throughput computational discovery of In2Mn2O7 as a high Curie temperature ferromagnetic semiconductor for spintronics*, npj computational materials, 5, 72, 2019

11 G. Brunin, G.-M. Rignanese, **G. Hautier**, *High-performance transparent conducting oxides through small-polaron transport*, Physical Review Materials, 3, 064602, 2019

12 J. J. de Pablo, N. E. Jackson, M. A. Webb, L.-Q. Chen, J. E. Moore, D. Morgan, R. Jacobs, T. Pollock, D. G. Schlom, E. S. Toberer, J. Analytis, I. Dabo, D. M. DeLongchamp, G. A. Fiete, G. M. Grason, **G. Hautier**, Y. Mo, K. Rajan, E. J. Reed, E. Rodriguez, V. Stevanovic, J. Suntivich, K. Thornton and J.-C. Zhao, *New frontiers for the materials genome initiative*, npj computational materials, 5, 41, 2019

13 I. T. Witting, T. C. Chasapis, F. Ricci, M. Peters, N. A. Heinz, **G. Hautier**, and J. G. Snyder, *The thermoelectric properties of bismuth telluride*, Advanced Electronic Materials, 5, 1800904, 2019

14 **G. Hautier**, *Finding the needle in the haystack: Materials discovery and design through computational ab initio high-throughput screening*, Computational Materials Science, 163, 108-116, 2019

15 J. J. Kuo, U. Aydemir, J.-H. Pöhls, F. Zhou, G. Yu, A. Faghaninia, F. Ricci, M. A. White, G.-M. Rignanese, **G. Hautier**, A. Jain and G. J. Snyder, , *Origins of ultralow thermal conductivity in 1-2-1-4 quaternary selenides*, Journal of Materials Chemistry A, 7, 2589-2596, 2019

16 V.-A. Ha, G. Yu, F. Ricci, D. Dahliah, M. J van Setten, M. Giantomassi, G.-M. Rignanese, **G. Hautier**, *Computationally-driven, high throughput identification of CaTe and LiSb as promising candidates for high mobility -type transparent conducting materials*, Physical Review Materials, 3, 034601, 2019

17 F. Naccarato, F. Ricci, J. Suntivich, **G. Hautier**, L. Wirtz, G.-M. Rignanese, *Searching for Materials with High Refractive Index and Wide Band Gap: A First-Principles High-Throughput Study*, Physical Review Materials, 3, 044602, 2019

18 D.-Y. Kuo, H. Paik, J. Kloppenburg, B. Faeth, K. M. Shen, D. G. Schlom, **G. Hautier** and J. Suntivich, *Measurements of Oxygen Electroadsorption Energies and Oxygen Evolution Reaction on RuO2(110): A Discussion of the Sabatier Principle and its Role in Electrocatalysis*, accepted in Journal of the American Chemical Society, 140, 17597-17605, 2018

19 L. A. Burton, F. Ricci, G.-M. Rignanese, **G. Hautier**, *High-Throughput Identification of Electrides from all Known Inorganic Materials* , Chemistry of Materials, 30, 7521-7526, 2018

20 J.-H. Pöhls, Z. Luo, U. Aydemir, J.-P. Sun, S. Hao, J. He, I. G. Hill, **G. Hautier**, A. Jain, C. Wolverton, G. J. Synder, H. Zhu, M. A. White, *Comparison between First-Principle Calculations and Experimental Studies of XYZ2 Thermoelectric Compounds* , Journal of Materials Chemistry A, 6, 19502, 2018

21 A. Lherbier, G. Vander Marcken, B. Van Troeye, A. Rafael Botello-Méndez, J.-J. Adjizian, **G. Hautier**, X. Gonze, G.-M. Rignanese, and J.-C. Charlier *Lithiation properties of sp2 carbon allotropes* , Physical Review Materials, 2, 085408, 2018

22 S. P. Ramkumar, A. Miglio, M. J. van Setten, D. Waroquiers, **G. Hautier**, and G. -M. Rignanese *Insights into cation disorder and phase transitions in CZTS from a first-principles approach* , Physical Review Materials, 2, 085403, 2018

23 W. Peng, G. Petretto, G.-M. Rignanese, **G. Hautier**, and A. Zevalkink *An Unlikely Route to Low Lattice Thermal Conductivity: Small Atoms in a Simple Layered Structure*, Joule, 2, 1879-1893, 2018

24 G. Petretto, S. Dwaraknath, H. P.C. Miranda, D. Winston, M. Giantomassi, M. J. van Setten, X. Gonze, K. A. Persson, **G. Hautier**, G.-M. Rignanese *High-throughput density-functional perturbation theory phonons for inorganic materials*, Scientific Data, 5, 180065, 2018

25 D. Broberg, B. Medasani, N. Zimmermann, G. Yu, A. Canning, M. Haranczyk, M. Asta, **G. Hautier**, *PyCDT: A Python toolkit for modeling point defects in semiconductors and insulators*, Computer Physics Communications, 226, 165-179, 2018

26 G. Petretto, X. Gonze, **G. Hautier**, G.-M. Rignanese, *Convergence and pitfalls of density functional perturbation theory phonons calculations from a high-throughput perspective*, Computational Materials Science, 144, 331-337, 2018

27 D.-Y. Kuo, C. J. Eom, J. K. Kawasaki, G. Petretto, J. N Nelson, **G. Hautier**, E. J. Crumlin, K. M. Shen, D. G. Schlom, J. Suntivich, *Influence of Strain on the Surface-Oxygen Interaction and the Oxygen Evolution Reaction of SrIrO3*, The Journal of Physical Chemistry C, 122, 4359-4364, 2018

28 N. Tumanova, N. Tumanov, K. Robeyns, F. Fischer, L. Fusaro, F. Morelle, V. Ban, **G. Hautier**, Y. Filinchuk, J. Wouters, T. Leyssens, F. Emmerling,*Opening Pandora's Box: Chirality, Polymorphism, and Stoichiometric Diversity in Flurbiprofen/Proline Cocrystals* , Crystal Growth & Design, 18, 954-961, 2018

29 N. Dardenne,**G. Hautier**, J.F. Gohy, J. Charlier, and G.-M. Rignanese *Ab initio calculations of open cell voltage in newly designed ptma-based li-ion organic radical batteries*, Computational materials science, 143, 27-31, 2018

30 S. Maier, S. Ohno, G. Yu, S. D. Kang, T. C. Chasapis, V. A. Ha, S. A. Miller, D. Berthebaud, M. G. Kanatzidis, G.-M. Rignanese, **G. Hautier**, G. J. Snyder, and F. Gascoin *Resonant Bonding, Multiband Thermoelectric Transport, and Native Defects in n-Type BaBiTe3–xSex (x = 0, 0.05, and 0.1)*, Chemistry of Materials, 30, 174-184, 2017

31 J.-H. Poehls, Z. Luo, U. Aydemir, J.-P. Sun, S. Hao, J. He, I. G. Hill, **G. Hautier**, A. Jain, X. Zeng, C. Wolverton, G. J. Snyder, H. Zhu, and M. A. White, *First-principles calculations and experimental studies of XYZ2 thermoelectric compounds: detailed analysis of van der Waals interactions*, Journal of Materials Chemistry A, 6, 19502-19519, 2018

32 M. Filip, X. Liu, A. Miglio, **G. Hautier**, F. Giustino, *Phase Diagrams and Stability of Lead-Free Halide Double Perovskites $Cs_2BB'X_6$, B = Sb, Bi, B' = Cu, Ag, Au and X = Cl, Br, I*, The Journal of Physical Chemistry C, 122, 158-170, 2017

33 J.-H. Poehls, A. Faghaninia, G. Petretto, U. Aydemir, F. Ricci, G. Li, M. Wood, S. Ohno, **G. Hautier**, G. J. Snyder, G.-M. Rignanese, A. Jain and M. A. White *Metal phosphides as potential thermoelectric materials*, Journal of Materials Chemistry C, 5, 12441-12456, 2017

34 M.J. van Setten, M. Giantomassi, X. Gonze, G.-M. Rignanese and **G. Hautier**, *Automation methodologies and large-scale validation for GW: Towards high-throughput GW calculations*, Physical Review B, 96, 155207, 2017

35 D. Waroquiers, X. Gonze, G.-M. Rignanese, C. Welker-Nieuwoudt, F. Rosowski, M. Goebel, S. Schenk, P. Degelmann, R. Andre, R. Glaum and **G. Hautier**, *Statistical analysis of coordination environments in oxides*, Chemistry of Materials, 29, 8346-8360, 2017

36 A. Miglio, C. P. Heinrich, W. Tremel, **G. Hautier** and W. G. Zeier, *Local bonding influence on the band edge and band gap formation in quaternary chalcopyrites*, Advanced Science, 4, 1700080, 2017

37 F. Ricci, W. Chen, U. Aydemir, G.J. Snyder, G.-M. Rignanese, A. Jain, **G. Hautier**, *Large scale database of electronic transport properties for inorganic crystalline compounds*, Scientific Data, 4, 170085, 2017

38 V.-A. Ha, F. Ricci, G.-M. Rignanese, **G. Hautier**, *Structural design principles for low hole effective mass s-orbital-based p-type oxides*, Journal of Materials Chemistry C, 5, 5772-5779, 2017

39 A. Faghaninia, G. Yu, U. Aydemir, M. Wood, W. Chen, G.-M. Rignanese, G. Jeffrey Snyder, **G. Hautier**, and A. Jain, *A computational assessment of the electronic, thermoelectric, and defect properties of bournonite (CuPbSbS3) and related substitutions*, Physical Chemistry Chemical Physics, 19, 6743-6756, 2017

40 D.-Y. Kuo, J. K. Kawasaki,J. N. Nelson, J. Kloppenburg **G. Hautier**, K. M. Shen, D. G. Schlom and J. Suntivich , *Influence of Surface Adsorption on the Oxygen Evolution Reaction on IrO2(110)*, Journal of the American Chemical Society, 139, 3473-3479, 2017

41 J. Varley, A. Miglio, V.-A. Ha, M. Van Setten, G.-M. Rignanese, **G. Hautier**, *High-throughput design of non-oxides p-type transparent conducting materials: data mining, search strategy and identification of boron phosphide*, Chemistry of Materials, 29, 2568-2573, 2017

42 Z. M. Gibbs, F. Ricci, G. Li, H. Zhu, K. Persson, G. Ceder, **G. Hautier**, A. Jain, G. J. Snyder, *Effective mass and Fermi Surface Complexity Factor from Ab- Initio Band Structure Calculations*,Npj Computational Materials, 3, 8, 2017

43 W. Sun, S. Dacek, S. P. Ong, **G. Hautier**, A. Jain, W. Richards, K. A. Persson, G. Ceder, *The Thermodynamic Scale of Inorganic Crystalline Metastability*, Science Advances, 2, e1600225, 2016

44 V.-A. Ha, D. Waroquiers, G.-M. Rignanese, **G. Hautier**, *Influence of the "second gap' on the transparency of transparent conducting oxides: an ab initio study*, Applied Physics Letters, 108, 201902, 2016

45 Wolfgang G. Zeier, J. Schmidt, **G. Hautier**, U. Aydemir, Z.M. Gibbs, C. Felser, G. J. Snyder, *Engineering half-Heusler thermoelectric materials using Zintl chemistry*, Nature Review Materials, 1, 16032, 2016

46 A. Jain, **G. Hautier**, S.P. Ong, K. Persson, *New opportunities for materials informatics: Resources and data mining techniques for uncovering hidden relationships*, Journal of Materials Science, 31, 977, 2016

47 W. Chen, J.-H. Pöhls, **G. Hautier**, D. Broberg, S. Bajaj, U. Aydemir, Z. M. Gibbs, H. Zhu, M. Asta, G. J. Snyder, B. Meredig, M. A. White, K. Persson and A. Jain, , *Understanding thermoelectric properties from high-throughput calculations: trends, insights, and comparisons with experiment*, Journal of Materials Chemistry C, 4, 4414-4426, 2016

48 I. Petousis, W. Chen, **G. Hautier**, T. Graf, T. D. Schladt, K. A. Persson, and F. B. Prinz, , *Benchmarking density functional perturbation theory to enable high-throughput screening of materials for dielectric constant and refractive index*, Physical Review B, 93,115151, 2016

49 R. Tang, Y. Nie, J. K. Kawasaki, D.-Y. Kuo, G. Petretto, **G. Hautier**, G.-M. Rignanese, K. M. Shen, D. G. Schlom and J. Suntivich , *Oxygen Evolution Reaction Electrocatalysis on $SrIrO_3$ epitaxially grown using Molecular Beam Epitaxy*, Journal of Materials Chemistry A, 4, 6831-6836

50 U. Aydemir, J.-H. Pohls, H. Zhu, **G. Hautier**, S. Bajaj, Z. M. Gibbs, W. Chen, G. Li, S. Ohno, D. Broberg, S. D. Kang, M. Asta, G. Ceder, M. A. White, K. Persson, A. Jain and G. J. Snyder *YCuTe2: a member of a new class of thermoelectric materials with CuTe4-based layered structure*, Journal of Materials Chemistry A, 4, 2461

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91 **G. Hautier**, J. D'Haen, K. Maex and P.M. Vereecken, *Electrodeposited free-standing single-crystal indium nanowire*, Electrochem. Solid-State Lett., 11(4): K47-K49, 2008

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Invited Talks

1 **G. Hautier** *Adsorption Energetics and Surface Phase Transformations in Iridium and Ruthenium-Based Oxygen Evolution Reaction Catalyst*, Materials Research Society, Boston, USA, November 2019

2 **G. Hautier** *Searching for materials with exceptional optical, electronic and spin properties using ab initio high-throughput computing*, 3rd Forum of Materials Genome Engineering, Kunming, China, November 2019

3 **G. Hautier** *Searching for materials with exceptional optical, electronic and spin properties using ab initio high-throughput computing*, seminar at the Sokolov Institute of Technology, Moscow, Russia, November 2019

4 **G. Hautier** *Searching for new Transparent Conducting and Electride Materials using high-throughput computational screening* , 11th International Symposium on Transparent Oxide and Related Materials for Electronics and Optics, Nara, Japan, October 2019

5 **G. Hautier** *High-throughput computational materials discovery and the Materials Project* , hands on DFT and beyond: high-throughput screening and big data analytics towards exascale computational materials science, Barcelona, Spain, September 2019

6 **G. Hautier** *Antimonides as thermoelectrics: the surprising electronic transport of Yb14MnSb11 and thermal conductivity of Mg3Sb2*, ICMAT 2019, Singapore, June 2019

7 **G. Hautier** *Searching for high performance p-type transparent conducting materials using high-throughput computing*, ICMAT 2019, Singapore, June 2019

8 **G. Hautier** *Combining density functional theory and experiments to understand and discover new solid-state electrolytes and oxygen evolution reaction catalysts*, CECAM Workshop Electrochemical Storage: Theory meets Industry, , Paris, France, June 2019

9 **G. Hautier** *Benchmarking DFT and beyond-DFT methods for thermodynamics and electronic properties* , Workshop on Precision Quantification in DFT, , Louvain-la-Neuve, Belgium, May 2019

10 **G. Hautier** *Building and browsing ab initio computational databases in quest of materials with exceptional opto-electronic properties*, American Physical Society March Meeting, , Boston, USA, March 2019

11 **G. Hautier** *Identifying materials with exceptional electronic properties using high-throughput computing and data mining*, seminar at the Max Planck Institute Stuttgart , Germany, November 2018

12 **G. Hautier** *Finding the needle in the haystack: Materials discovery through high-throughput ab initio computing and data mining*, 9th International Conference on Multiscale Materials Modeling (MMM2018) , Osaka, Japan, November 2018

13 **G. Hautier** *Opportunities and challenges in high-throughput computing*, CECAM NOMAD summer school , Lausanne, Switzerland, September 2018

14 **G. Hautier** *Finding the Needle in a Haystack: Materials discovery through high-throughput ab initio computing and data mining*, UC Davis department of Chemistry seminar , Davis, USA, September 2018

15 **G. Hautier** *Finding the Needle in a Haystack: Materials discovery through high-throughput ab initio computing and data mining*, Leverhulme Research Centre for Functional Materials Design Inaugural Symposium , Liverpool, UK, September 2018

16 **G. Hautier** *New materials discovery through high-throughput screening and data mining*, seminar at the Materials Science Department of Nanyang Technological University (NTU), Singapore, July 2018

17 **G. Hautier** *Superionic conduction through frustrated energy landscape*, 12th International Conference on Ceramic Materials and Components for Energy and Environmental Applications (CMCEE 2018), Singapore, July 2018

18 **G. Hautier** *New materials discovery through high-throughput screening and data mining*, CECAM workshop on machine learning at interfaces, Lausanne, Switzerland, June 2018

19 **G. Hautier** *High-throughput ab initio screening for exceptional materials*, Symposium on Chemical Bonding in the 21st century organized in honor of Prof. Roald Hoffmann, Brussels, Belgium, May 2018

20 **G. Hautier** *Accelerating new materials discovery through ab initio computing, high-throughput screening and data mining*, seminar at the University Frederico II, Naples, Italy, May 2018

21 **G. Hautier** *A Combined Theory-Experiment Study of the Surface Oxygen Adsorption and Oxygen Evolution Reaction on Well-Defined Iridium Oxide Catalysts*, MRS Spring 2018, Phoenix, USA, April 2018

22 **G. Hautier** *Superionic conduction through frustrated energy landscape*, MRS Spring 2018, Phoenix, USA, April 2018

23 **G. Hautier** *Materials Discovery through high-throughput ab initio computing and data mining*, MRS Spring 2018, Phoenix, USA, April 2018

24 **G. Hautier** *Finding the Needle in a Haystack: Materials discovery through high-throughput ab initio computing and data mining*, MaX Conference on the Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing, Trieste, Italy, January 2018

25 **G. Hautier** *Ab initio-driven computational search and design of new materials*, seminar at the Ecole Polytechnique, Palaiseau, France, January 2018

26 **G. Hautier** *Finding the Needle in a Haystack: Materials discovery through high-throughput ab initio computing and data mining*, seminar at the Vrije Universiteit Brussels (VUB), Brussels, Belgium, November 2017

27 **G. Hautier** *Finding the Needle in a Haystack: Materials discovery through high-throughput ab initio computing and data mining*, Heraeus seminar-ab initio Electronic Structure Theory for Solids in the 21st Century, Bad Honnef, Germany, October 2017

28 **G. Hautier** *A brief (and surely biased) overview of first principles computations in Li-ion battery electrodes and solid electrolytes*, Theory meets Experiment - Battery Materials, Giessen, Germany, October 2017

29 **G. Hautier** *Speeding up materials discovery through ab initio computing and high-throughput screening*, Giessen University Chemistry Seminar, Giessen, Germany, October 2017

30 **G. Hautier** *High-throughput computational search for new high mobility p-type transparent (semi)conducting materials*, TCO Leipzig 2017, Leipzig, Germany, September 2017

31 **G. Hautier** *Everything you wanted to know about DFT in Li-ion batteries (but were too afraid to ask)*, Summer group retreat Janek/Gasteiger groups, Monte Isola, Italy, September 2017

32 **G. Hautier** *Finding the Needle in a Haystack: Materials Discovery through high-throughput ab initio computing and data mining*, 53rd Symposium on Theoretical Chemistry (STC), Basel, Switzerland, August 2017

33 **G. Hautier** *High-throughput computational search for new high mobility p-type transparent (semi)conducting materials*, 10th International Conference on the Science and Technology for Advanced Ceramics (STAC-10), Yokohama, Japan, August 2017

34 **G. Hautier** *High-throughput computational search for new high mobility p-type transparent (semi)conducting materials*, 10th International Symposium on Transparent Oxide and Related Materials for Electronics and Optics (TOEO-10), Tokyo, Japan, July 2017

35 **G. Hautier** *Finding the needle in the haystak: Materials Discovery through high-throughput ab initio computing and data mining*, Pennsylvania State University Materials Science and Engineering Department seminar, State College, USA, May 2017

36 **G. Hautier** *Finding the needle in the haystak: Materials Discovery through high-throughput ab initio computing and data mining*, Cornell Materials Science and Engineering Department seminar, Ithaca, USA, February 2017

37 **G. Hautier** *Finding the Needle in a Haystack: A High-Throughput Computational Approach to Materials Discovery*, German Science Foundation Summer School on solar fuels, Berlin, Germany, September 2016

38 **G. Hautier** *Accelerating the discovery of high mobility transparent (semi)conducting oxides through high-throughput computing*, European Materials Research Society Fall meeting, Warsaw, Poland, September 2016

39 **G. Hautier** *Finding the Needle in a Haystack: A High-Throughput Computational Approach to Materials Discovery*, ICTMC-20 conference, Halle, Germany, September 2016

40 **G. Hautier** *Accelerating materials discovery through high-throughput computing and data mining*, AiiDA workshop, Lausanne, Switzerland, June 2016

41 **G. Hautier** *High-throughput computational search for transparent conducting and thermoelectric materials*, E-MRS Spring Meeting, Lille, France, April 2016

42 **G. Hautier** *Finding the needle in a haystack through high-throughput ab initio computing*, seminar at the Materials Science and Engineering Department of the Massachusetts Institute of Technology (MIT), Cambridge, USA, April 2016

43 **G. Hautier** *Speeding up materials discovery and bringing informatics to solid state chemistry through high-throughput ab initio computing*, seminar at Bonn University, Bonn, Germany, December 2015

44 **G. Hautier** *Finding the material needle in the haystack through high-throughput ab initio computing*, seminar at the theory department of the Fritz Haber Institute (FHI), Berlin, Germany, November 2015

45 **G. Hautier** *Finding the material needle in the haystack through high-throughput ab initio computing*, seminar at Materials Department Oxford University, Oxford, UK, October 2015

46 **G. Hautier** *Speeding up materials discovery through high-throughput ab initio computing*, seminar at the Ruhr University, Bochum, Germany, October 2015

47 **G. Hautier** *High-Throughput Ab Initio Computations for Li-Ion Batteries: Materials Identification and Data Mining* , 8th International Conference on Materials for Advanced Technologies of the Materials Research Society of Singapore (ICMAT2015), Singapore, June 2015

48 **G. Hautier** *Prediction of new battery materials based on ab initio calculations - the materials project*, 2nd International Freiberg Conference on Electrochemical Storage Materials (ESTORM), Freiberg, Germany, June 2015

49 **G. Hautier** *High-throughput computational search for new high mobility transparent (semi)conducting oxides* , American Physical Society meeting, San Antonio, USA, March 2015

50 **G. Hautier** *Finding the material needle in the haystack: high-throughput computational screening as an accelerator to materials discovery* , seminar at Delft University, Netherlands, February 2015

51 **G. Hautier** *Searching for New High Performance Materials with ab initio High-Throughput Computing*, seminar at the Université de Montréal, Canada, December 2014

52 **G. Hautier** *High-throughput computations as an accelerator for materials discovery: an application to p-type transparent conducting oxides*, seminar at the University of Bath, UK, August 2014

53 **G. Hautier** *Searching for high mobility p-type transparent conducting oxides using high-throughput computations* , seminar in Professor Chris Van de Walle's group at the University of California Santa Barbara (UCSB), Santa Barbara, USA, June 2014

54 **G. Hautier** *Accelerating materials discovery through high-throughput ab initio computing*, seminar at the nano engineering Department, University of California San Diego (UCSD), San Diego, USA, April 2014

55 **G. Hautier** *Accelerating materials discovery through high-throughput ab initio computing*, seminar at the Materials Science Department Cornell University, Ithaca, USA, April 2014

56 **G. Hautier** *High-throughput ab initio computing for molecular and materials design*, Institute of Condensend Matter and Nanosience seminar, Louvain-la-Neuve, Belgium, March 2014

57 **G. Hautier** *High-throughput computations as an accelerator for materials discovery: an application to p-type transparent conducting oxides*, International workshop on computational physics and materials science, Lausanne, Switzerland, January 2014

58 **G. Hautier** *High-throughput computations as an accelerator for materials discovery: an application to p-type transparent conducting oxides*, CRP-Gabriel Lippmann, Belvaux, Luxemburg, December 2013

59 **G. Hautier** *Accelerating materials discovery through high-throughput computing and the Materials Project*, Departement Metaalkunde en Toegepaste Materiaalkunde KU Leuven seminar, Leuven, Belgium, November 2013

60 **G. Hautier** *High-throughput computations as an accelerator for materials discovery: an application to p-type transparent conducting oxides*, Seminar at the Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany, November 2013

61 **G. Hautier** *High-throughput computations as an accelerator for materials discovery: an application to p-type transparent conducting oxides*, Seminar at Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany, October 2013

62 **G. Hautier** *Accelerating materials discovery through high-throughput computing and the Materials Project*, Special Seminar at Unicat (German cluster of excellence in catalysis), Berlin, Germany, September 2013

63 **G. Hautier** *A new Klondike for materials? The Materials Project*, Materials Evolution workshop, Lund, Sweden, September 2013

64 **G. Hautier** *A High-Throughput Computational Search for New p-type Transparent Conducting Oxides*, Workshop on The future of transparent conducting oxides, Hasselt, Belgium, June 2013

65 **G. Hautier** *Data Mined Compound and Crystal Structure Prediction for High-Throughput Materials Discovery*, Society for Industrial and Applied Mathematics (SIAM) conference on Mathematical aspects of Materials Science, Philadelphia, USA, June 2013

66 **G. Hautier** *Accelerating materials discovery for industrial applications using high-throughput ab initio computing*, European Theoretical Spectroscopy Facility (ETSF) Young researchers' meeting, Budapest, Hungary, May 2013

67 **G. Hautier** *Finding new p-type Transparent Conducting Oxides through high-throughput computations*, seminar in Prof. Ceder's group at Massachusetts Institute of Technology, Cambridge, MA, USA, March 2013

68 **G. Hautier** *Accelerating new (earth-abundant) materials discovery through high-throughput computing*, workshop on Sustainable and Resource-Efficient Materials, Uppsala, Sweden, December 2012

69 **G. Hautier** *The Materials Project: A Database of High-Throughput Ab Initio Computed Data*, CECAM workshop on Validation and Verification in Electronic-Structure calculations: state of the art and perspectives, Lausanne, Switzerland, September 2012

70 **G. Hautier** *High-Throughput Computational Identification of New Lithium-Ion Battery Cathode Materials*, seminar at the Interuniversity Microelectronics Centre (IMEC), Heverlee, Belgium, June 2012

71 **G. Hautier** *Using first principles computations to understand, discover and design Li-ion battery cathode materials*, European Theoretical Spectroscopy Facility (ETSF) Young researchers' meeting, Brussels, Belgium, May 2012

72 **G. Hautier** *Predicting New Materials Using the Substitution Predictor*, Materials Research Society Spring meeting, San Francisco, USA, April 2012

73 **G. Hautier** *High-throughput ab initio computations for materials design and the Materials Project Database*, Trends in Nanotechnology (TNT) 2011, Tenerife, Spain, November 2011

74 **G. Hautier** *High-throughput Computational Search of New Materials and its Application to Lithium-ion Batteries*, Interdisciplinary Center for Advanced Materials Simulation (ICAMS), Bochum, Germany, November 2011

75 **G. Hautier**, G. Ceder *High-throughput computational identification of new lithium-ion battery cathode materials*, 242nd American Chemical Society (ACS) Meeting, Denver, CO, August 2011

76 **G. Hautier** *Accelerated New Materials Discovery through High-Throughput Ab initio Computing and its Application to Lithium-Ion Batteries*, Fourth International Workshop on Combinatorial Materials Research, Ghent, Belgium, June 2011

77 **G. Hautier** *Combining data mining and high-throughput ab initio computations for new materials discovery*, Computing Sciences Seminar, Berkeley National Laboratory, USA, April 2011

78 **G. Hautier**, A. Jain, C. Moore, C. Fischer, T. Mueller, H. Chen, R. Doe and G. Ceder *High-throughput ab initio computations for accelerated new materials discovery and its application to lithium-ion batteries*, Chemistry of Novel Materials Laboratory Seminar, Université Mons-Hainaut, Belgium, June 2010

79 **G. Hautier**, A. Jain, C. Moore, C. Fischer, T. Mueller, H. Chen, R. Doe and G. Ceder *High-throughput ab initio computations for accelerated new materials discovery and its application to lithium-ion batteries*, Professor Xavier Gonze's group seminar, Université catholique de Louvain, Belgium, June 2010

80 **G. Hautier**, A. Jain, C. Moore, C. Fischer, T. Mueller, H. Chen, R. Doe and G. Ceder *High-throughput ab initio computations for accelerated new materials discovery*, Electronic-structure challenges in materials modeling for energy applications, CECAM workshop, Lausanne, Switzerland, June 2010

81 **G. Hautier**, C. C. Fischer, A. Jain and G. Ceder *Combining data mining and high-throughput ab initio computations for new materials discovery*, Materials Modelling Laboratory seminar, Oxford University, UK, November 2009

Contributed Talks

AS PRESENTING AUTHOR

1 W. Chen, J. George, J. Varley, G.-M. Rignanese, **G. Hautier** *High-throughput computational discovery of In2Mn2O7 pyrochlore oxide as a high curie temperature ferromagnetic semiconductor for spintronics* , Materials Research Society Fall Meeting, Boston, USA, November 2018

2 **G. Hautier**, D. Waroquiers, X. Gonze, G.-M. Rignanese, C. Welker-Nieuwoudt, F. Rosowski, M. Goebel, S. Schenk, P. Degelmann, R. Andre, R. Glaum *Large Scale Data Mining of Coordination Environments in Oxides* , Materials Research Society Fall Meeting, Boston, USA, November 2018

3 **G. Hautier**, D. Di Stefano, A. Miglio, K. Robeyns, Y. Filinchuk, M. Lechartier, A. Senyshyn, H. Ishida, S. Spannenberger, M. Wilkening, B. Roling, Y. Kato, *Very High Lithium Diffusion in LiTi2(PS4)3 Through Energy Landscape Frustration*, Materials Research Society Fall Meeting, Boston, USA, November 2018

4 **G. Hautier**, D. Di Stefano, A. Miglio, K. Robeyns, Y. Filinchuk, M. Lechartier, A. Senyshyn, H. Ishida, S. Spannenberger, M. Wilkening, B. Roling, Y. Kato *Superionic conduction through frustrated energy landscape* , Materials Research Society (MRS) Fall, Boston, USA, November 2017

5 **G. Hautier**, J. Varley, A. Miglio, V.-A. Ha, G.-M. Rignanese *High-throughput computational search for new high performance transparent (semi)conducting materials* , European Materials Research Society Spring Meeting, Strasbourg, France, May 2017

6 **G. Hautier**, D. Waroquiers, X. Gonze, G.-M. Rignanese, C. Welker-Nieuwoudt, F. Rosowski, M. Goebel, S. Schenk, P. Degelmann, R. Andre, R. Glaum *High-Throughput Detection and Data Mining of Coordination Environments in Oxides* , Materials Research Society Spring Meeting, Phoenix, USA, April 2017

7 **G. Hautier**, J. Varley, A. Miglio, V.-A. Ha, G.-M. Rignanese *High-throughput computational search for new high mobility transparent (semi)conducting materials* , Materials Research Society Spring Meeting, Phoenix, USA, April 2017

8 **G. Hautier**, J. Varley, A. Miglio, V.-A. Ha, G.-M. Rignanese *High-throughput computational search for new high mobility transparent (semi)conducting materials* , DPG Spring Meeting, Dresden, Germany, December 2017

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