Personal data

Date of birth: 4 February, 1985
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Scientific profile

Ivano E. Castelli currently leads a group of 7 people working in the field of quantum mechanical simulations for materials discovery. During the last ten years, his research focused on the design of novel materials for sustainable energy applications using Density Functional Theory (DFT) simulations and artificial intelligence (AI) techniques as well as on develop methodologies to accelerate the materials discovery. He often collaborates with experimental groups and companies to elucidate materials properties at the atomic level. His research interests include:

- Development of workflows and machine learning techniques to automate the design of novel materials
- High-throughput screening for novel materials in the reduced dimensionality realm (2D and 1D)
- Modeling of solid/liquid (Li-ion batteries, molten salt reactors) and solid-solid interfaces
- Design of electrochemical reconfigurable materials
- Identification of descriptors and use of machine learning techniques applied to materials design
- Perovskites and pyrochlores for light harvesting, water splitting, and oxygen evolution reaction

Education and Personal Experience

09/2017	Assistant Professor, DTU Energy, Technical University of Denmark, DK.
09/2015	Post Doc., Department of Chemistry (Rossmeisl group), University of Copenhagen, DK.
09/2014	EPFL Post Doc. Fellow, Theory and Simulation of Materials (Marzari group), EPFL, CH.
06/2013	Post Doc., Center for Atomic-scale Materials Design (Jacobsen group), DTU Physics, DK.
26/09/2013	Ph.D. degree, thesis title *Computational Screening of Materials for Water Splitting Applications.*
03/2012	Visiting Ph.D. student, Suncat (Nørskov group), SLAC, Stanford, USA.
06/2010	Ph.D. student, Center for Atomic-scale Materials Design (Jacobsen Group), Department of Physics, Technical University of Denmark, DK.
10/2007	M.Sc. student, Department of Physics, Università degli Studi di Milano, I.
10/2004	B.Sc. student, Department of Physics, Università degli Studi di Milano, I.

Grants

2021 - 2024	Independent Research Fund Denmark (Tematic Call - Green Transition, Proj 1), *Reconfigurable Metamaterials for Next Generation High-capacity Batteries* (PI, 2.88M DKK).
2021	DTU Energy, *Design and Printing of Solid State Batteries* (PI, 400K DKK).
2020 - 2021	Danish ERC Programme, *Multiscale Design of Electrochemical Metamaterials* (PI, 338K DKK).
2020 - 2023	EU - H2020, *BATTERY 2030+ Large-scale Research Initiative* (co-PI, share: 300K DKK).
2020 - 2023	EU - H2020, *Battery Interface Genome - Materials Acceleration Platform* (co-PI, 1.2M DKK).
2020 - 2022	Innovation Fund Denmark (Industrial Postdoc), *Quantum Chemical Modelling of Molten Salt Interfaces Corrosion* (academic PI, 240K DKK).
2020	DTU LearningLab, *Virtual Laboratory Framework for the Discovery of Energy Materials* (PI, 300K DKK).
2020	DTU Energy, *3D Printing and Design of Solid State Batteries* (PI, 800K DKK).
2019 - 2021	Independent Research Fund Denmark (Proj 1), *Triple-Conducting Electrocatalysts Enabling Miniaturized Solid Oxide Fuel Cells to Power Internet of Things* (co-PI, 200K DKK).
2018 - 2021	BMW Group, *Computational Study of the Solid Electrolyte Interface Formation* (co-PI, 675K DKK).
2018 - 2021	DTU Energy, *Autonomous Materials Discovery* (co-PI, 1.2M DKK).
2018	DTU Energy, *Lithium Storage in Hybrid and Inorganic Perovskites* (PI, 575K DKK).
2015	EPFL Fellows co-funded by Marie Skłodowska-Curie (CE-COFUND Fellow - Fund 587704), *Computational Materials Design of Novel Perovskites for Photocatalytic Water Splitting and for the Oxygen Evolution Reaction* (PI, 650K DKK).

Qualifications and Awards

2020	**Under evalutaion** for promotion to Associated Professor. Updates available at http://www.ivca.eu/evaluation.pdf.
2020	**Abilitazione Scientifica Nazionale** Professore di Prima Fascia FIS02/B2 - Fisica Teorica della Materia (Abilitation as full professor of theorical condensed matter physics for the Italian minister of university and research).
2020	**Selected** for the second stage of the *ERC Starting Grant 2020* (grade A, fundable but prioritize differently.
2020	**Selected** for the second stage of the *DFF - Sapere Aude Starting Grant 2020*.
2019	**Selected** for the second stage of the *DFF - Sapere Aude Starting Grant 2019*.
2019	Nominated **Emerging Leader 2020** by the editorial board of *J. Phys.: Energy*.

Commissions of Trust

2021 -	**Substitute Member** of the Study Board, DTU Energy, DK.
2021 -	**Pedagogical Coordinator**, DTU Energy, DK.
2020 - 2021	**Member** of *Working Group for Department Innovation Strategy*, DTU Energy, DK.
2021 -	**Editorial Board** of *Modelling, Theory and Computational Catalysis* (Frontiers in Catalysis).
2020 -	**Co-author** of *Roadmap: Inventing the Sustainable Batteries of the Future*.
2020 -	**Advisory Board** of *Challenges* (MDPI).
2019 - 2020	**Member** of *Working Group for Department Strategy*, DTU Energy, DK.
2019 -	**Editorial Board** of *Materials* and *Materials Proceedings* (MDPI).
2018 -	**Ambassator** for pilot project *Well-being for scientific staff*, DTU Energy, DK.
2016 - 2017	**Member** of *Junior Investigator Network 2016* and *Alumni*, Copenhagen University, DK.
2014 - 2015	**Member** of *MX Library Committee*, EPFL, CH.

Reviewer

2019	**External Ph.D. exam**: opponent for one Ph.D. defence at University of Bern, CH.
2019	**Scientific evaluator**: grant-proposal reviewer for the Icelandic Research Fund.
2012 -	**Reviewer** for more than 25 journals (Nature group, American Chemical Society, Royal Chemistry Society, American Institute of Physics, Wiley, Springer, Elsevier, Institute of Physics, MDPI).

Management Experience

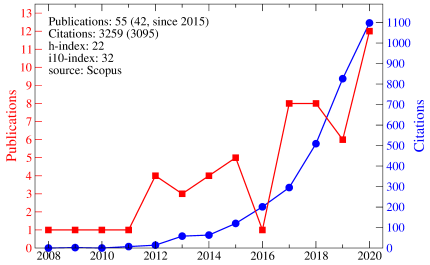
2021	**Project Manager** of *Design and Printing of Solid State Batteries*, DTU Energy.
2020 - 2023	**Data Management Responsible** of *Battery Interface Genome - Materials Acceleration Platform*, EU-H2020.
2020	**Project Manager** of *Virtual Laboratory Framework for the Discovery of Energy Materials*, DTU LearningLab.
2020	**Project Manager** of *3D Printing and Design of Solid State Batteries*, DTU Energy.
2018 - 2021	**co-PI** of *Computational Study of the Solid Electrolyte Interface Formation*, BMW Group.
2018 - 2021	**WP Leader** of *Second-life of Data, Autonomous Materials Discovery (AiMade)*, DTU Energy.
2018	**Project Manager** of *Lithium Storage in Hybrid and Inorganic Perovskites*, DTU Energy.

Organization of Scientific Meetings

2020	**Battery2030+ Research Data Management**, Battery 2030+ Consortium.
2020	**DTU Energy Talks** for students, MSc Programme, DTU.
2019, 2022	**E-MRS Spring Meeting**, *Computations for materials - discovery, design and the role of data.*
2019	**BATMAN Summer School**, Hillerød, DK.
2015	**MARVEL Junior Retreat**, Männedorf, CH.

Dissemination Summary

Peer reviewed articles: 55 (43 senior publications);
First author: 20 (12); **Last author:** 3 (3); **Corresponding author:** 19 (17);
Leading computational author in first-author experimental papers: 26 (23);
2 Published patents; **4 Chapters** in books;
6 Highly cited papers; **1 hot papers** (source Web of Science);
6 Cover pages in peer reviewed journals; **3 Open source databases**;
3259 Citations; **22 h-index**; **32 i10-index** (source Scopus);
24 Invited talks; $>$ **50 Contributed talks and posters**.



Supervision Experience

When main supervisor is indicated with *.

• Postdoc

2021 - 2023 * To be hired.
2020 - 2022 Eibar Flores.
2020 - 2022 * Luca Silvioli.
2020 - 2021 * Katrine Louise Svane.
2019 - 2021 Haiwu Zhang, coordination of the computational activities.

• Ph.D. students

2020 - 2023 Kai Zheng, *Quantum Mechanical Simulations for an Autonomous Discovery of Energy Materials* (China Scholarship Council Fellow).
2018 - 2021 Zhenyun Lan, *Computational Design of Perovskite-based Materials for Sustainable Energy Applications* (China Scholarship Council Fellow).
2018 - 2021 August Edwards Guldberg Mikkelsen, *Accelerating Clean Energy Materials Discovery from Second-life of Data.*
2018 - 2021 Felix Tim Bölle, *Machine Learning and Ab-initio Simulations for Accelerated Materials Discovery.*

• Research assistants

2019 * Peter Ebert Christensen.
2018 * August Edwards Guldberg Mikkelsen.

• Master student

2021 * Andrea Fedrigucci, *Autonomous Search of Solid-state Electrolytes with Antiperovskite Symmetry.*
2021 * Benjamin Sjølin, *Modelling Nickel Doping to Enhance Resistance against Sodium Hydroxide.*
2015 - 2016 Thomas Anthony Andreas Batchelor, *A Density-Functional Theory Study to Determine the Potential of a High Entropy Alloy, PtPdIrRuRh, as a Surface for Catalysis.*

• Bachelor students

2021 * Alexandra Craft Ludvigsen, *New Photoferroic Layered Perovskites for Photoelectrochemical Water Splitting.*
2020 * Jacob Lamp Matthiessen, *Antiperovskites: a New Class of Materials for a Sustainable Future.*
2020 * Nestor Chatenet, *Autonomous Design of Cathode Materials for Efficient Multivalent Batteries.*
2019 * Alexander Juul Nielsen, *High-throughput Screening of Cathode Materials for Efficient Mg-Intercalation and Diffusion.*
2018 Peter Ebert Christensen, *Machine Learning Based Prediction of 3D to 2D Structure Transitions in Energy Materials.*
2016 Mathias Dam Spo, *Trends in Adsoprtion Energy on p− and n−type TiO_2.*

Teaching Experience

Teaching Qualification: Diploma University Teaching, UDTU, H33 (March 2019). **Line Responsible**: *Future Energy*, bachelor in *General Engineering*, DTU. **Course Responsible**: Autonomous Materials Discovery (DTU, MSc, 5 ECTS, June 2020); Computational modelling of materials for energy applications (DTU, MSc, 5 ECTS, Fall 2019 and 2020); Computational modelling of materials for energy applications (DTU, MSc, 5 ECTS, Fall 2018); **Course co-Responsible**: Electrochemical Energy Technologies (DTU, MSc, 5 ECTS, June 2020); **Special Courses**: EuroteQ Challenges (EuroteQ Univ., MSc, 5 ECTS, Summer 2021); Computational modelling of materials for energy applications (DTU, PhD, 5 and 10 ECTS, Spring 2020 and 2021); Design of Energy Metamaterials (DTU, BSc, 10 ECTS, Fall 2019); Photoferroic Materials for Electrocatalytic Reactions (DTU, MSc, 5 ECTS, Fall 2017), Data Mining in Perovskites (DTU, MSc, 5 ECTS, Spring 2014), Calculation of Absorption Spectra Using Time-Dependent Density Functional Theory (DTU, MSc, 5 ECTS, Jan. 2012). **Lectures**: BATMAN - Battery Modeling & Advanced Numerical Simulations 2019; Joint European Summer School (JESS) 2017, 2018 and 2019 (Athens, Greece); Advanced Computational Tools for Energy Materials (DTU, Fall 2017 and 2018); Battery Materials and Chemistries: from Fundamental Mechanisms to Battery Cells (DTU, Fall 2017 and 2018); Sustainable Chemistry (University of Copenhagen, Spring 2016 and 2017). **Superuser**: DTU Learn (From 2020).

Active International Collaborations

USA: Dr. Nenad M. Markovic (Argonne Nat. Lab.), Prof. Yang Shao-Horn (MIT), Prof. Vladan Stevanovic (Colorado School of Mines), Prof. Wissam A. Saidi (Pittsburgh University), Prof. Shubhra Bansal (University of Nevada); **Germany**: Dr. Filippo Maglia (BMW Reasearch Group); **Switzerland**: Prof. Nicola Marzari (EPFL), Prof. Thomas J. Schmidt (ETHZ, PSI), Prof. Thomas Lippert (PSI); **Czech Republic**: Dr. Petr Krtil (Czech Academy of Sciences); **France**: Dr. Stephan Bourdais (IMRA Europe); **China**: Prof. Yongfeng Wang (Peking University); **Israel**: Prof. Reshef Tenne (Weizmann Institute of Science); **Europe**: EU-H2020 Battery2030+ and BIG-MAP consortia.

List of Publications - Ivano E. Castelli

Articles in Peer-reviewed Journals
Selected significant publications are marked with a ***** and corresponding author publications with †. IEC contribution for the most significant publications is also reported. Scopus is used to count the number of citations (only ≥ 100 is indicated).

Total number of citations: 3259; h-index: 22; i10-index: 32.

55. B.-J. Kim, E. Fabbri, M. Borlaf, D. F. Abbott, **I. E. Castelli**, M. Nachtegaal, T. Graule, and T. J. Schmidt, Oxygen Evolution Reaction Activity and Underlying Mechanism of Perovskites Electrocatalysts at Differnt pH, *Mater. Adv.*, DOI: 10.1039/D0MA00661K (2020).

54. R. K. Pittkowski, D. F. Abbott, R. Nebel, S. Divanis, E. Fabbri, **I. E. Castelli**, T. J. Schmidt, J. Rossmeisl, and P. Krtil, Synergistic Effects in Oxygen Evolution Activity of Mixed Iridium-ruthenium Pyrochlores, *Electrochimica Acta* **366**, 137327 (2021).

53. H. Zhang, **I. E. Castelli**,† S. Santucci, S. Sanna, N. Pryds, and V. Esposito, Atomic-scale Insights into Electrosteric Substitutional Chemistry of Cerium Oxide, *Phys. Chem. Chem. Phys.* **22**, 21900 (2020).

52. D. Schwartz, R. Murshed, H. Larson, B. Usprung, S. Soltanmohamad, R. Pandey, E. S. Barnard, A. Rockett, T. Hartmann, **I. E. Castelli**,† and S. Bansal, Air Stable, High-Efficiency, Pt-Based Halide Perovskite Solar Cells with Long Carrier Lifetimes, *Phys. Status Solidi RRL* **2020**, 2000182 (2020).

51. V. Esposito and **I. E. Castelli**,† Metastability at Defective Metal Oxide Interfaces and Nanoconfined Structures, *Adv. Mater. Interfaces* **2020**, 1902090 (2020).

50. M. Liang, W. Lin, Z. Lan, J. Meng, Q. Zhao, X. Zou, **I. E. Castelli**, T. Pullerits, S. Canton, K. Zheng, Electronic Structure and Trap-States of Two-Dimensional Ruddlesden-Popper Perovskites with Relaxed Goldschmidt Tolerance Factor, *ACS Applied Electronic Materials* **2**, 1402 (2020).

49. J. Meng, Z. Lan, M. Abdellah, B. Yang, S. Mossin, M. Liang, M. Naumova, Q. Shi, S. Gutierrez Alvarez, Y. Liu, W. Lin, **I. E. Castelli**, S. Canton, T. Pullerits, and K. Zheng, Modulating Charge Carrier Dynamics in Mn-Doped All-inorganic Halide Perovskite Quantum Dots through the Doping-Induced Deep Trap States, *J. Phys. Chem. Lett.* **11**, 3705 (2020).

48. ***** W. A. Saidi, W. Shadid, and **I. E. Castelli**, Machine-Learning Structural and Electronic Properties of Metal Halide Perovskites Using a Hierarchical Convolutional Neural Network, *npj Computational Materials* **6**, 36 (2020). Contribution: definition of a convolutional neural network and relevant features to describe and predict band gap in hybrid halide perovskites.

47. *** I. E. Castelli**,† M. Zorko, T. M. Østergaard, P. Martins, P. P. Lopes, B. K. Antonopoulos, F. Maglia, N. Markovic, D. Strmcnik, and J. Rossmeisl, The Role of an Interface in Stabilizing Reaction Intermediates for Hydrogen Evolution in Aprotic Electrolytes, *Chem. Sci.* **11**, 3914 (2020). Contribution: new methodology to model the SEI interface and new insight into the reduction reactions of impurities.

46. S.Sanna, E. Fiordaliso, T. Kasama, **I. E. Castelli**, and V. Esposito, Effect of high oxygen deficiency in nanoconfined bismuth sesquioxide, *J.Phys.: Energy* **2**, 024010 (2020).

45. ***** F. T. Bölle, N. R. Mathiesen, A. J. Nielsen, T. Vegge, J. M. Garcia Lastra, and **I. E. Castelli**,† Autonomous Discovery of Materials for Intercalation Electrodes, *Batteries & Supercaps* **3**, 488 (2020). Contribution: design of a comprehensive workflow to identify intercalation electrodes based on thermodynamic and kinetic properties.

44. **I. E. Castelli**,† T. Olsen, Y. Chen, Towards Photoferroic Materials by Design: Recent Progresses and Perspective, *J.Phys.: Energy* **2**, 011001 (2020).

43. W. Si, Z. P. Tehrani, F. Haydous, N. Marzari, **I. E. Castelli**, D. Pergolesi, and T. Lippert, *Yttrium Tantalum Oxynitride Multiphases as Photoanodes for Water Oxidation*, *J. Phys. Chem. C* **123**, 26211 (2019).

42. D. F. Abbott, R. K. Pittkowski, K. Macounova, R. Nebel, E. Marelli, E. Fabbri, **I. E. Castelli**,† P. Krtil, T. J. Schmidt, Design and Synthesis of Ir/Ru Pyrochlore Catalysts for the Oxygen Evolution Reaction Based on Their Bulk Thermodynamic Properties, *ACS Appl. Mater. Interfaces*, 11, 37748 (2019).

41. A. Bhowmik, **I. E. Castelli**, J. M. Garcia-Lastra, P. B. Jørgensen, O. Winther, and T. Vegge, A Perspective on Inverse Design of Battery Interphases using Multi-scale Modelling, Experiments and Generative Deep Learning, *Energy Storage Materials* **21**, 446 (2019).

40. B.-J. Kim, E. Fabbri, **I. E. Castelli**, M. Borlaf, T. Graule, M. Nachtegaal, and T. J. Schmidt, Fe-Doping in Double Perovskite $PrBaCo_{2(1-x)}Fe_{2x}O_{6-\delta}$: Insights into Structural and Electronic Effects to Enhance Oxygen Evolution Catalyst Stability, *Catalysis* **9**, 263 (2019).

39. B.-J. Kim, E. Fabbri, D. F. Abbott, X. Cheng, A. H. Clark, M. Nachtegaal, M. Borlaf, **I. E. Castelli**, T. Graule, and T. J. Schmidt, Functional Role of Fe-Doping in Co-Based Perovskite Oxide Catalysts for Oxygen Evolution Reaction, *J. Am. Chem. Soc.* **141**, 5231 (2019).

38. T. A.A. Batchelor, J. K. Pedersen, S. H. Winther, **I. E. Castelli**, K. W. Jacobsen, and J. Rossmeisl, High-Entropy Alloys as a Discovery Platform for Electrocatalysis, *Joule* **3**, 834 (2019).

37. ***** G. Prandini,‡ A. Marrazzo,‡ **I. E. Castelli**,‡, N. Mounet, and N. Marzari, Precision and Efficiency in Solid-state Pseudopotential Calculations, *npj Computational Materials* **4**, 72 (2018). ‡ Contributed equally. Contribution: design of the benchmark protocol based on structural and electronic properties.

36. B.-J. Kim, X. Cheng, D. Abbott, E. Fabbri, F. Bozza, T. Graule, **I. E. Castelli**, L. Wiles, N. Danilovic, K. E. Ayers, N. Marzari, and T. J. Schmidt, Highly Active Nanoperovskite Catalysts for Oxygen Evolution Reaction: Insights into Activity and Stability of $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_{2+\delta}$ and $PrBaCo_2O_{5+\delta}$, *Advanced Functional Materials* **28**, 1804355 (2018).

35. X. Cheng, E. Fabbri, Y. Yamashita, **I. E. Castelli**, B. Kim, M. Uchida, R. Haumont, I. Puente-Orench, and T. J. Schmidt, Oxygen Evolution Reaction on Perovskites: A Multieffect Descriptor Study Combining Experimental and Theoretical Methods, *ACS Catal.* **8**, 9567 (2018).

34. **I. E. Castelli**, S. G. Soriga, and I. C. Man, Effects of the Cooperative Interaction on the Diffusion of Hydrogen on MgO(100), *J. Chem. Phys.* **149**, 034704 (2018).

33. T. Østergaard, L. Giordano, **I. E. Castelli**, F. Maglia, B. K. Antonopoulos, Y. Shao-Horn, and J. Rossmeisl, Oxidation of Ethylene Carbonate on Li Metal Oxide Surfaces, *J. Chem Phys C* **122**, 10442 (2018).

32. ***** D. Strmcnik, **I. E. Castelli**, J. G. Connell, D. Haering, M. Zorko, P. Martins, P. P. Lopes, B. Genorio, T. Østergaard, H. Gasteiger, F. Maglia, B. K. Antonopoulos, V. R. Stamenkovic, J. Rossmeisl, and N. M. Markovic, Electrocatalytic Transformation of Impurity HF to H_2 and LiF in Lithium Ion Batteries, *Nature Catalysis* **1**, 255 (2018). Contribution: simulations of the solid-electrolyte interface and understanding of the formation of the LiF layer at the atomic scale.

31. N. Mounet, M. Gibertini, P. Schwaller, D. Campi, A. Merkys, A. Marrazzo, T. Sohier, **I. E. Castelli**, A. Cepellotti, G. Pizzi, and N. Marzari, Two-dimensional Materials from High-throughput Computational Exfoliation of Experimentally Known Compounds, *Nature Nanotechnology* **13**, 246 (2018). Cited: 481 times.

30. A. Fluri, E. Gilardi, M. Karlsson, V. Roddatis, M. Bettinelli, **I. E. Castelli**, T. Lippert, and D. Pergolesi, Anisotropic Proton and Oxygen Ion Conductivity in Epitaxial $Ba_2In_2O_5$ Thin Films, *J. Phys. Chem. C* **121**, 21797 (2017).

29. **I. E. Castelli**, I. C. Man, S.-G. Soriga, V. Parvulescu, N. B. Halck, and J. Rossmeisl, The Role of the Band Gap for the Interaction Energy of Coadsorbed Fragments, *J. Phys. Chem. C* **121**, 18608 (2017).

28. M. E. Björketun, **I. E. Castelli**,† J. Rossmeisl, T. Olsen, K. Ukai, M. Kato, G. Dennler, and K. W. Jacobsen, Defect Chemistry and Electrical Conductivity of Sm-doped $La_{1-x}Sr_xCoO_{3-\delta}$ for Solid Oxide Fuel Cells, *J. Phys. Chem. C* **121**, 15017 (2017).

27. D. Lebedev, M. Povia, K. Waltar, P. M. Abdala, **I. E. Castelli**, E. Fabbri, M. V. Blanco, A. Fedorov, C. Coperet, N. Marzari, and T. J. Schmidt, Highly Active and Stable Iridium Pyrochlores for Oxygen Evolution Reaction, *Chemisty of Materials* **29**, 5182 (2017).

26. A. H. Larsen, J. J. Mortensen, J. Blomqvist, **I. E. Castelli**, R. Christensen, M. Dułak, J. Friis, M. N. Groves, B. Hammer, C. Hargus, E. D. Hermes, P. C. Jennings, P. Bjerre Jensen, J. Kermode, J. R. Kitchin, E. L. Kolsbjerg, J. Kubal, S. Lysgaard, J. Bergmann Maronsson, T. Maxson, T. Olsen, L. Pastewka, A. Peterson, C. Rostgaard, J. Schiøtz, O. Schütt, M. Strange, K. Thygesen, T. Vegge, L. Vilhelmsen, M. Walter, Z. Zeng, and K. W. Jacobsen, The Atomic Simulation Environment - A Python Library for Working with Atoms, *J. Phys.: Condens. Matter* **29**, 273002 (2017). Cited: 632 times.

25. M. Pichler, J. Szlachetko, **I. E. Castelli**, N. Marzari, M. Döbeli, A. Wokaun, D. Pergolesi, and T. Lippert, Determination of Conduction and Valence Band Electronic Structure of $LaTiO_xN_y$ Thin Film, *ChemSusChem* **10**, 2099 (2017).

24. B.-J. Kim, D. F. Abbott, X. Cheng, E. Fabbri, M. Nachtegaal, F. Bozza, **I. E. Castelli**, D. Lebedev, R. Schäublin, C. Copéret, T. Graule, N. Marzari, and T. J. Schmidt, Unraveling Thermodynamics, Stability, and Oxygen Evolution Activity of Strontium Ruthenium Perovskite Oxide, *ACS Catalysis* **7**, 3245 (2017).

23. K. M. Macounova, M. Klusáčková, R. Nebel, M. Zukalova, M. Klementova, **I. E. Castelli**, M. D. Spo, J. Rossmeisl, L. Kavan, and P. Krtil, The Synergetic Surface Sensitivity of Photo-Electrochemical Water Oxidation on TiO_2 (Anatase) Electrodes, *The Journal of Physical Chemistry C* **121**, 6024 (2017).

22. K. Lejaeghere, G. Bihlmayer, T. Björkman, P. Blaha, S. Blügel, V. Blum, D. Caliste, **I. E. Castelli**, S. J. Clark, A. Dal Corso, S. de Gironcoli, T. Deutsch, J. K. Dewhurst, I. Di Marco, C. Draxl, M. Dułak, O. Eriksson, J. A. Flores-Livas, K. F. Garrity, L. Genovese, P. Giannozzi, M. Giantomassi, S. Goedecker, X. Gonze, O. Grånäs, E. K. U. Gross, A. Gulans, F. Gygi, D. R. Hamann, P. J. Hasnip, N. A. W. Holzwarth, D. Iuşan, D. B. Jochym, F. Jollet, D. Jones, G. Kresse, K. Koepernik, E. Küçükbenli, Y. O. Kvashnin, I. L. M. Locht, S. Lubeck, M. Marsman, N. Marzari, U. Nitzsche, L. Nordström, T. Ozaki, L. Paulatto, C. J. Pickard, W. Poelmans, M. I. J. Probert, K. Refson, M. Richter, G.-M. Rignanese, S. Saha, M. Scheffler, M. Schlipf, K. Schwarz, S. Sharma, F. Tavazza, P. Thunström, A. Tkatchenko, M. Torrent, D. Vanderbilt, M. J. van Setten, V. Van Speybroeck, J. M. Wills, J. R. Yates, G.-X. Zhang, and S. Cottenier, Reproducibility in Density Functional Theory Calculations of Solids, *Science* **351** (6280), 1415 (2016). Cited 503 times. Contribution: design of the procedure to test pseudopotential libraries in Quantum Espresso.

21. ***** X. Cheng, E. Fabbri, M. Nachtegaal, **I. E. Castelli**, M. El Kazzi, R. Haumont, N. Marzari, and T. J. Schmidt, Oxygen Evolution Reaction on $La_{1-x}Sr_xCoO_3$ Perovskites: A Combined Experimental and Theoretical Study of Their Structural, Electronic, and Electrochemical Properties, *Chem. Mater.* **27**, 7662 (2015). Cited 138 times. Contribution: insight in the electrocatalytic properties by correlating bulk descriptors to surface properties.

20. **I. E. Castelli**,† K. S. Thygesen, and K. W. Jacobsen, Calculated Optical Absorption of Different Perovskite Phases, *J. Mater. Chem. A* **3**, 12343 (2015).

19. **I. E. Castelli**,† M. Pandey, K. S. Thygesen, and K. W. Jacobsen, Bandgap Engineering of Functional Perovskites Through Quantum Confinement and Tunneling, *Phys. Rev B* **91**, 165309 (2015).

18. H. Li, **I. E. Castelli**, K. S. Thygesen, and K. W. Jacobsen, Strain Sensitivity of Band Gaps of Sn-Containing Semiconductors, *Phys. Rev B* **91**, 045204 (2015).

17. **I. E. Castelli**,† F. Hüser, M. Pandey, H. Li, K. S. Thygesen, B. Seger, A. Jain, K. Persson, G. Ceder, and K. W. Jacobsen, New Light Harvesting Materials Using Accurate and Efficient Bandgap Calculations, *Advanced Energy Materials* **5**, 1400915 (2015).

16. **I. E. Castelli**,† J. M. García-Lastra, K. S. Thygesen, and K. W. Jacobsen, Bandgap Calculations and Trends of Organometal Halide Perovskites, *APL Mater.* **2**, 081514 (2014). Cited 124 times.

15. B. Seger, **I. E. Castelli**, P. C. K. Vesborg, K. W. Jacobsen, O. Hansen, and I. Chorkendorff, 2-Photon Tandem Device for Water Splitting: Design Parameters and Feasibility, *Energy & Environmental Science* **7**, 2397 (2014).

14. **I. E. Castelli**† and K. W. Jacobsen, Designing Rules and Probabilistic Weighting for Fast Materials Discovery in the Perovskite Structure, *Modelling Simul. Mater. Sci. Eng.* **22**, 055007 (2014).

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Pre-prints

- ***** K. L. Svane, S. Z. Lefmann, M. S. Vilmann, J. Rossmeisl, and **I. E. Castelli**, *The Influence of the Artificial Nanostructure on the LiF Formation at the Solid-electrolyte Interphase of Carbon-based Anodes*, *ChemRxiv*, DOI: 10.26434/chemrxiv.13332464, under review in *ACS Applied Energy Materials*. Contribution: definition and supervision of the project, analysis of the data.
- ***** F. T. Bölle, A. E. G. Mikkelsen, K. S. Thygesen, T. Vegge, and **I. E. Castelli**, *Structural and Chemical Mechanisms Governing Stability of Inorganic Janus Nanotubes*, *arXiv*, DOI: 2011.14708, under review in *npj Comp. Mater.* Contribution: definition and supervision of the project, analysis of the data.
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Patents

- ***** *High electrically conducting current collector ceramic material for SOFC*, number: JP, 2017-157553 (granted, 2017). Contribution: DFT study of stable and conductive perovskites.
- *High electrically conducting current collector ceramic material for SOFC*, number: EP 3211703(A1) (application, 2017).
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Chapters in Books

- A. Bhowmik, F. T. Bölle, **I. E. Castelli**, J. H. Chang, J. M. García-Lastra, N. R. Mathiesen, A. S. Tygesen, and T. Vegge, Generation of Computational Data Sets for Machine Learning Applied to Battery Materials in *Atomic-Scale Modelling of Electrochemical Systems*, ed. K. Laasonen, T. Laurila, and M. Melander, Wiley, in printing (2020). ISBN: 9781119605614
- A. Bagger, **I. E. Castelli**, M. H. Hansen, and J. Rossmeisl, Fundamental Atomic Insight in Electrocatalysis in *Handbook of Materials Modeling*, ed. W. Andreoni and S. Yip, Springer, July 2018.
- *** I. E. Castelli**,† K. Kuhar, M. Pandey, and K. W. Jacobsen, Computational Screening of Light-Absorbing Materials for Photoelectrochemical Water Splitting in *Advances in Photoelectrochemical Water Splitting*, ed. D. Tilley, S. Lany and R, van de Krol, RSC Editor, February 2018. Contribution: main writing contribution, screening studies for light harvesting materials, identification of different levels of descriptors and implementation of computational tools used to select candidate materials.
- **I. E. Castelli**,† K. S. Thygesen, and K. W. Jacobsen, Computational High-throughput Screening for Solar Energy Materials in *Theoretical Modeling of Organohalide Perovskites for Photovoltaic Applications*, ed. G. Giorgi and K. Yamashita, CRC Press, June 2017.

Non-peer-reviewed Publications

- Inventing the Sustainable Batteries of the Future, https://battery2030.eu/research/roadmap/
- A. H. Larsen, J. J. Mortensen, J. Blomqvist, **I. E. Castelli**, R. Christensen, M. Dułak, J. Friis, M. N. Groves, B. Hammer, C. Hargus, E. D. Hermes, P. C. Jennings, P. Bjerre Jensen, J. Kermode, J. R. Kitchin, E. L. Kolsbjerg, J. Kubal, S. Lysgaard, J. Bergmann Maronsson, T. Maxson, T. Olsen, L. Pastewka, A. Peterson, C. Rostgaard, J. Schiøtz, O. Schütt, M. Strange, K. Thygesen, T. Vegge, L. Vilhelmsen, M. Walter, Z. Zeng, and K. W. Jacobsen, The Atomic Simulation Environment - A Python Library for Working with Atoms, Ψ_k *Scientific Highlight of The Month* **No. 134**, January 2017.

Cover Pages

- *J. Phys.: Condens. Matter* **24**, 104019 (2012)
- *APL Materials* **2**, 081514 (2014)
- *Advanced Energy Materials* **5**, 1400915 (2015)
- *Nature Nanotechnology* **13**, 246 (2018)
- *Adv. Mater. Interfaces* **2020**, 1902090 (2020)
- *Batteries & Supercaps* **3**, 488, (2020)

Databases

- ***** Novel perovskite for light harvesting:
  http://cmr.fysik.dtu.dk/
  Contribution: 25000 materials for visible light harvesting. This includes inorganic and metal-organic perovskites in different crystal phases as well as experimentally known materials from other databases. The database has been

established in 2012 and I have started multiple collaborations thanks to sharing of the data collected in it.
- Pseudopotential verification and the Standard Solid State Pseudopotential library:
  http://materialscloud.org/sssp/
  Contribution: protocol and data to benchmark 10 pseudopotential libraries for the Quantum Espresso package. Since its development in 2015, this database has been visited more than 500 time a month.
- Trends and catalysis:
  http://nano.ku.dk/english/research/theoretical-electrocatalysis/katladb/
  Contribution: structures and scripts related with different projects from catalysis on oxides to molecular dynamic structures for the investigation of the solid-liquid electrolyte in Li-ion batteries. The database has been established in 2017.

Invited Talks and Seminars

Most significant presentations are marked with a *.
- *TBA*
  53rd Heyrovsky Discussion, 2021.
- *Towards an Accelerated Design of Battery Materials and Interfaces*
  Dipartimanto di Fisica, Università degli Studi di Milano, Nov. 19, 2020.
- **Accelerated Discovery of Battery Electrodes using an Automatic Workflow, Topology Criteria and Machine Learning*
  Batt&Supercaps Webinar Series, Oct. 13 - 14, 2020.
- *Accelerated Design of Hybrid Halide Perovskites*
  Computation of Halide Perovskites, Sep. 8 - 9, 2020.
- **How to Autonomously Design Better Battery Materials and Interfaces using Density Functional Theory*
  ARTISTIC Project Webinar Series, Jun. 29 - Jul. 3, 2020.
- **The Role of Electrochemical Interface in Stabilizing Reaction Intermediates for H_2 Evolution and SEI Formation in Aprotic Electrolyte*
  Battery2030+ Web Conference, May 25 - 26, 2020.
- *Atomic-scale Modeling of Materials for Solid Oxide Cells*
  44^{th}th International Conference and Exposition on Advanced Ceramics and Composites (ICACC 2020), Daytona Beach, Florida, USA, Jan 26 - 31, 2020.
- ***Atomic-scale Modeling of Materials with Reduced Dimensionality and Interfaces*
  International Conference on Electroceramics - Oxide materials at low dimensional limit: Surfaces and interfaces, Lausanne, Switzerland, Jul 14 - 19, 2019.
- *Atomic Scale Understanding of the SEI Formation in Li-ion Batteries*
  IDA Energy Week, Copenhagen, Denmark, May 23, 2018.
- *Understand and Predict Properties of Materials at the Atomic Scale*
  J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic, Dec. 7, 2017.
- ***Pourbaix Diagrams and Electrochemical Stability for the OER*
  Final RENERG^2 Project Conference, EMPA Academy, Dübendorf, Switzerland, Oct. 30, 2017.
- *High-throughput Screening of Ceramic Materials for Light Absorption*
  15th Conference & Exhibition of the European Ceramic Society, Budapest, Hungary, Jul. 9 - 13, 2017.
- *Electrochemical Interface at the Atomic Scale - Water and the LP57 Electrolytes*
  eMRS 2016 Spring, Lille, France, May. 2 - 6, 2016.
- *Theory and Experiment Synergy for Artificial Photosynthesis* and *Development of Advanced Electrocatalysts for Water Splitting: Correlation between Electronic Structure, Surface Properties and Electrochemical Activity*
  MARVEL PP7 Day, PSI, Villigen, Switzerland, Mar. 3, 2016.
- *Verification of Pseudopotential Libraries - The Standard Solid State Pseudopotentials*
  QuantumWise, Copenhagen, Denmark, Nov. 3, 2015.
- *Verification of Pseudopotential Libraries - The Standard Solid State Pseudopotentials*
  CAMd, DTU, Kgs. Lyngby, Denmark, Sep. 24, 2015.
- ***Bandgap Calculations and Trends of Hybrid Halide Perovskites*
  CECAM Workshop: Perovskite solar cells: the quest for a theoretical description, CECAM-HQ-EPFL, Lausanne, Switzerland, Aug. 25 - 28, 2015.
- *High-throughput Computational Screening of Perovskite Oxides and Related Compounds for Light Harvesting Applications*
  PSI, Villigen, Switzerland, Oct. 6, 2014.
- *High-throughput Screening of New Materials for Water Splitting Applications*
  EPFL, Lausanne, Switzerland, May 5, 2014.
- *Computational Screening of Materials for Water Splitting Applications*
  Cornell University, Ithaca, New York, USA, Nov. 25, 2013.
- *High-throughput Screening of New Materials for Water Splitting Applications*
  SLAC National Accelerator Laboratory, Menlo Park, California, USA, Oct. 23, 2013.
- *High-throughput Screening of New Materials for Water Splitting Applications*
  Lawrence Berkeley National Laboratory, Berkeley, California, USA, Oct. 22, 2013.

– *High-throughput Screening of New Materials for Water Splitting Applications*
Workshop II, Fuels from Sunlight, Los Angeles, California, USA, Oct. 14 - 18, 2013.