Ivano E. Castelli

Contact Information

Section for Atomic Scale Modelling and Materials, DTU Energy, Department of Energy Conversion and Storage. Fysikvej, Building 309, Office 146, Technical University of Denmark - DK 2800, Kgs. Lyngby, Denmark.
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Scopus Author ID: 25821783000
ResearcherID: N-1627-2015
Google Scholar: https://scholar.google.dk/citations?user=cUJuTxkAAAAJ&

Employment

From 2017, Sep. - Assistant Professor at DTU Energy, Section for Atomic Scale Modelling and Materials, Department of Energy Conversion and Storage, Technical University of Denmark - DK 2800, Kgs. Lyngby, Denmark.

2015, Sep. - 2017, Aug. - Post Doc. at Department of Chemistry, University of Copenhagen Ø - DK 2100, Copenhagen, Denmark.

2014, Sep. - 2015, Aug. - Post Doc. (EPFL Fellow) at Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne - CH 1015, Lausanne, Switzerland.

2013, Jun. - 2014, Aug. - Post Doc. at Center for Atomic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark - DK 2800, Kgs. Lyngby, Denmark.

Funding

- 2015, Feb. - 2015, Aug. - EPFL Fellows co-funded by Marie Skłodowska-Curie (COFUND Fellow - Fund 587704).
- 2018, Jan. - DTU Energy, Technology Track Batteries, *Lithium Storage in Hybrid and Inorganic Perovskites* - PI, 575k DKK.

Education

2013, Sep. 26 - Ph.D. Degree in Physics at the Center for Atomic-scale Materials Design (CAMD), Department of Physics, Technical University of Denmark - Kgs. Lyngby, Denmark.

- Thesis title: *Computational Screening of Materials for Water Splitting Applications.*
- Supervisors: K. W. Jacobsen (Technical University of Denmark), K. S. Thygesen (Technical University of Denmark)
- http://dcwww.camd.dtu.dk/~ivca/phd_thesis.pdf
- http://dcwww.camd.dtu.dk/~ivca/phd_presentation.pdf

2012, Mar - External stay at Suncat, SLAC, Stanford (California) with Prof. Jens K. Nørskov.

2010, Apr. 09 - Master Degree in Physics at the Università degli Studi di Milano - Milano, Italy, with full marks.

- Thesis title: *Structural and Magnetic Properties of sp-Hybridized Carbon.*
- Supervisors: N. Manini (Milano University), G. Onida (Milano University)

- http://materia.fisica.unimi.it/manini/theses/castelliMag.pdf

2007, Oct. 25 - Bachelor Degree in Physics at the Università degli Studi di Milano - Milano, Italy, with full marks.

- Thesis title: *Quantized Lubrican Velocity in a Bi-Dimensional Sliding Model.*
- Supervisors: N. Manini (Milano University), R. Capozza (Modena and Reggio Emilia University)
- http://materia.fisica.unimi.it/manini/theses/castelli.pdf

1999, Sep. - 2004, Jun - Liceo Scientifico "G. B. Grassi" - Saronno, Italy, with mark of 100/100.

Publications

(The most significant publications are indicated with an *****)

32. *****_Electrocatalytic Transformation of Impurity HF to H_2 and LiF in Lithium Ion Batteries_, 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, accepted in *Nature Chemistry*.

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

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

29. *The Role of the Band Gap for the Interaction Energy of Coadsorbed Fragments*, I. E. Castelli, Isabela-Costinela Man, Stefan-Gabriel Soriga, Vasile Parvulescu, Niels Bendtsen Halck, and Jan Rossmeisl, *J. Phys. Chem. C* **121**, 18608 (2017).

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

27. *Highly Active and Stable Iridium Pyrochlores for Oxygen Evolution Reaction*, 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, *Chemisty of Materials* **29**, 5182 (2017).

26. *****_The Atomic Simulation Environment - A Python Library for Working with Atoms_, 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, *J. Phys.: Condens. Matter* **29**, 273002 (2017).

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

24. *Unraveling Thermodynamics, Stability, and Oxygen Evolution Activity of Strontium Ruthenium Perovskite Oxide*, 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, *ACS Catalysis* **7**, 3245 (2017).

23. *The Synergetic Surface Sensitivity of Photo-Electrochemical Water Oxidation on TiO_2 (Anatase) Electrodes*, 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 Journal of Physical Chemistry C* **121**, 6024 (2017).

22. *The Atomic Simulation Environment - A Python Library for Working with Atoms*, 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, Ψ_k *Scientific Highlight of The Month* **No. 134**, January 2017.

21. ***Reproducibility in Density Functional Theory Calculations of Solids**, 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, *Science* **351** (6280), 1415 (2016).

20. *Oxygen Evolution Reaction on $La_{1-x}Sr_xCoO_3$ Perovskites: A Combined Experimental and Theoretical Study of Their Structural, Electronic, and Electrochemical Properties*, X. Cheng, E. Fabbri, M. Nachtegaal, I. E. Castelli, M. El Kazzi, R. Haumont, N. Marzari, and T. J. Schmidt, *Chem. Mater.* **27**, 7662 (2015).

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

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

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

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

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

14. ***2-Photon Tandem Device for Water Splitting: Design Parameters and Feasibility**, B. Seger, I. E. Castelli, P. C. K. Vesborg, K. W. Jacobsen, O. Hansen, and I. Chorkendorff, *Energy & Environmental Science* **7**, 2397 (2014).

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

12. *Calculated Pourbaix Diagrams of Cubic Perovskites for Water Splitting: A Critical Stability Analysis*, I. E. Castelli, K. S. Thygesen, and K. W. Jacobsen, *Topics in Catalysis* **57**, 265 (2014).

11. *Stability and Band Gaps of Layered Perovskites for One- and Two-photon Water Splitting*, I. E. Castelli, J. M. García-Lastra, F. Hüser, K. S. Thygesen, and K. W. Jacobsen, *New Journal of Physics* **15**, 105026 (2013).

10. ***Performance of Genetic Algorithms in Search for Water Splitting Perovskites*, A. Jain, I. E. Castelli, G. Hautier, D. H. Bailey, and K. W. Jacobsen, *Journal of Materials Science* **48**, 6519 (2013).

9. *Bandgap Engineering of Double Perovskites for One- and Two-Photon Water Splitting*, I. E. Castelli, K. S. Thygesen, and K. W. Jacobsen, *MRS Online Proceedings Library* **1523**, 2013.

8. *New Cubic Perovskites for One- and Two-Photon Water Splitting using the Computational Materials Repository*, I. E. Castelli, D. D. Landis, K. S. Thygesen, S. Dahl, I. Chorkendorff, T. F. Jaramillo, and K. W. Jacobsen, *Energy & Environmental Science* **5**, 9034 (2012).

7. *Mechanical Properties of Carbynes Investigated by Ab Initio Total-energy Calculations*, I. E. Castelli, P. Salvestrini, and N. Manini, *Phys. Rev. B* **85**, 214110 (2012).

6. ***Computational Screening of Perovskite Metal Oxides for Optimal Solar Light Capture*, I. E. Castelli, T. Olsen, S. Datta, D. D. Landis, S. Dahl, K. S. Thygesen, and K. W. Jacobsen, *Energy & Environmental Science* **5**, 5814 (2012).

5. *Carbon sp Chains in Graphene Nanoholes*, I. E. Castelli, N. Ferri, G. Onida, and N. Manini, *J. Phys.: Condens. Matter.* **24**, 104019 (2012).

4. *Vibrational Characterization of Dinaphthylpolyynes: A Model System for the Study of End-capped sp Carbon Chains*, E. Cinquanta, L. Ravagnan, I. E. Castelli, F. Cataldo, N. Manini, G. Onida, and P. Milani, *J. Chem. Phys.* **135**, 194501 (2011).

3. *Synthesis, Characterization and Modelling of Naphthyl-terminated sp-Carbon Chains: Dinaphthylpolyynes*, F. Cataldo, L. Ravagnan, E. Cinquanta, I. E. Castelli, N. Manini, G. Onida, and P. Milani, *J. Phys. Chem. B* **114**, 14834 (2010).

2. *Tribology of the Lubricant Quantized-sliding State*, I. E. Castelli, R. Capozza, A. Vanossi, G.E. Santoro, N. Manini, and E. Tosatti, *J. Chem. Phys.* **131**, 174711 (2009).

1. *Role of Transverse Displacements for a Quantized-velocity State of the Lubricant*, I. E. Castelli, N. Manini, R. Capozza, A. Vanossi, G. E. Santoro, and E. Tosatti, *J. Phys.: Condens. Matter* **20**, 354005 (2008).

Publications under Review

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

- *Highly Active Nano-Perovskite Catalysts for Oxygen Evolution Reaction: Insights into Activity and Stability in Alkaline and Quasi-Neutral pH Electrolytes*, K. Bae-Jung, X. Cheng, D. Abbott, F. Bozza, T. Graule, I. E. Castelli, ..., N. Marzari, and T. J. Schmidt, submitted to *Nano Energy.*

- *Oxygen Evolution Reaction on Perovskites: A Multi-Effect Descriptors Study Combining Experimental and Theoretical Methods*, X. Cheng, E. Fabbri, Y. Yamashita, I. E. Castelli, K. Bae-Jung, M. Uchida, R. Haumont, I. P. Orench, and T. J. Schmidt, submitted to *Joule.*

Patents

- *High electrically conducting current collector ceramic material for SOFC*: JP, 2016-037201 and JP, 2017-157553.
- *High electrically conducting current collector ceramic material for SOFC*: EP, 3211703 A1.

Chapters in Books

- *Computational High-throughput Screening for Solar Energy Materials*, I. E. Castelli, K. S. Thygesen, and K. W. Jacobsen, in *Theoretical Modeling of Organohalide Perovskites for Photovoltaic Applications*, ed. G. Giorgi and K. Yamashita, CRC Press, June 2017.
- *Computational Screening of Light-Absorbing Materials for Photoelectrochemical Water Splitting*, I. E. Castelli, K. Kuhar, M. Pandey, and K. W. Jacobsen, RSC Editor, in printing, 2018.
- *Electrocatalysis*, J. Rossmeisl, I. E. Castelli, A. Bagger, submitted, Fall 2017.

Cover Pages

- *J. Phys.: Condens. Matter* **24**, 104019 (2012): http://www.ivca.eu/images//cm2410-Mar2012.pdf
- *APL Materials* **2**, 081514 (2014): http://www.ivca.eu/images//APLMater_Aug2014.pdf
- *Advanced Energy Materials* **5**, 1400915 (2015): http://www.ivca.eu/images/AEM-Jan2015.pdf
- *Nature Nanotechnology* **13**, 246 (2018): http://www.ivca.eu/images/NatNanotech_March2018.png

Databases

- Novel perovskite for light harvesting: http://cmr.fysik.dtu.dk/
- Pseudopotential verification and the Standard Solid State Pseudopotential library: http://materialscloud.org/sssp/
- Trends and catalysis: http://nano.ku.dk/english/research/theoretical-electrocatalysis/katladb/

Invited Talks and Seminars

- *High-throughput Screening of New Materials for Water Splitting Applications*

  Workshop II, Fuels from Sunlight,

  Los Angeles, California, USA, Oct. 14 - 18, 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*

SLAC National Accelerator Laboratory, Menlo Park, California, USA, Oct. 23, 2013.

- *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*

  EPFL, Lausanne, Switzerland, May 5, 2014.

- *High-throughput Computational Screening of Perovskite Oxides and Related Compounds for Light Harvesting Applications*

  PSI, Villigen, Switzerland, Oct. 6, 2014.

- *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.

- *Verification of Pseudopotential Libraries - The Standard Solid State Pseudopotentials*

  CAMd, DTU, Kgs. Lyngby, Denmark, Sep. 24, 2015.

- *Verification of Pseudopotential Libraries - The Standard Solid State Pseudopotentials*

  QuantumWise, Copenhagen, Denmark, Nov. 3, 2015.

- *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.

- *Electrochemical Interface at the Atomic Scale - Water and the LP57 Electrolytes*

  eMRS 2016 Spring,

  Lille, France, May. 2 - 6, 2016.

- *High-throughput Screening of Ceramic Materials for Light Absorption*

  15th Conference & Exhibition of the European Ceramic Society

  Budapest, Hungary, Jul. 9 - 13, 2017.

- *Atomic-scale Modeling in Fuel Cell, Electrolyser and Battery Research*, *Transport Modeling in Batteries - Ionic and Electronic Transport*, and *Beyond Li-ion Batteries - Resource-efficient Batteries*

  JESS2017, Summer School

  Athens, Greece, Sep. 11 - 15, 2017.

- *Pourbaix Diagrams and Electrochemical Stability for the OER*

  Final RENERG^2 Project Conference

  EMPA Academy, Dübendorf, Switzerland, Oct. 30, 2017.

- *Understand and Predict Properties of Materials at the Atomic Scale*

  J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic, Dec. 7, 2017.

Conferences, Workshops and Meetings

- *Exactly Quantized Sliding of a Confined Solid Lubricant under Shear*

  ECOSS 26, European Conference on Surface Science,
  Parma, Italy, Aug. 30 - Sep. 4, 2009.

- *Exactly Quantized Sliding of a Confined Solid Lubricant under Shear*

  Joint ICTP/FANAS Conference on Trends in Nanotribology,
  Trieste, Italy, Oct. 19 - 24, 2009.

- ACAM- SFI SimBioMa-ESF Workshop: Molecular Friction,

  Dublin, Ireland, Dec. 14 - 16, 2009.

- *Electronic Structure and Vibrational Properties of Carbynes in Graphene Nanoholes*

  TransAlp'Nano 2010,
  Como, Italy, Jun. 3 - 5, 2010.

- CASE 2nd Annual Review Meeting,

  Helsinge, Denmark, Jun. 14 - 15, 2010.

- CAMD Summer School 2010

  Kgs. Lyngby, Denmark, Aug. 14 - 20, 2010.

- Ψ_K 2010 Conference

  Berlin, Germany, Sep. 12 - 16, 2010.

- *Computational Screening of Metal Oxides for Solar Cell Harvesting Materials*

  CAMd Meeting 2010,
  Magleaas Conference Center, Denmark, Nov. 8 - 9, 2010.

- *Computational Screening of Metal Oxides for Solar Cell Harvesting Materials*

  NanoDay 2010,
  Kgs. Lyngby, Denmark, Dec. 6, 2010.

- *Computational Screening of Metal Oxides for Solar Cell Harvesting Materials*

  European Graduate School on Sustainable Energy Technology,
  Nyborg, Denmark, Dec. 9 - 11, 2010.

- *Computational Screening of Perovskite Metal Compounds for Photocatalytic Water Splitting*

  Materials Informatics: Tools for Design and Discovery,
  CECAM-HQ-EPFL, Lausanne, Switzerland, May 23 - 25, 2011.

- *Computational Screening of Perovskite Metal Oxides for Solar Light Capture*

  CASE 3rd Annual Review Meeting,
  Klinten, Denmark, Sep. 15 - 16, 2011.

- *Computational Screening of Perovskite Metal Compounds for Photocatalytic Water Splitting*

  Photo-meets Electrocatalysis: United We Split (...Water),
  Delmenhorst, Germany, Oct. 4 - 7, 2011.

- CAMD Summer School 2012

  Kgs. Lyngby, Denmark, Aug. 18 - 24, 2012.

- *Double Perovskites for Single- and Two-Photon Water Splitting*

  Energy from the Sun: Computational Chemists and Physicists Take up the Challenge,

  Chia Laguna Resort, Italy, Sep. 10 - 14, 2012.

- *Cubic, Double, and Layered Perovskites for One- and Two-Photon Water Splitting*

  2012 MRS Fall Meeting & Exhibit,

  Boston, Massachusetts, USA, Nov. 25 - 30, 2012.

- *Layered Perovskites for One- and Two-photon Water Splitting*

  DPG Spring Meeting,

  Regensburg, Germany, Mar. 10 - 15, 2013.

- *Computational Screening of Perovskites for One- and Two-photon Water Splitting*

  Solar Energy for World Peace,

  Istanbul, Turkey, Aug. 17 - 19, 2013.

- *Computational Screening of Materials for Water Splitting Applications*

  2013 MRS Fall Meeting & Exhibit,

  Boston, Massachusetts, USA, Dic. 1 - 6, 2013.

- *Calculation of Pourbaix Diagrams Combining DFT and Experimental Data as Descriptor for High-Throughput Screening*

  DPG Spring Meeting,

  Dresden, Germany, Mar. 30 - Apr. 4, 2014.

- *High-throughput Screening of Materials for Water Splitting Applications* and *Designing Rules and Probabilistic Weighting for Fast Materials Discovery in the Perovskite Structure*

  eMRS 2014 Spring,

  Lille, France, May. 26 - 30, 2014.

- *Calculation of Pourbaix Diagrams as Descriptor for High-throughput Screening*

  65 Annual Meeting of the International Society of Electrochemistry,

  Lausanne, Switzerland, Aug. 31 - Sep. 5, 2014.

- *New Light-Harvesting Materials Using Accurate and Efficient Bandgap Calculations*

  Frontiers of First-principles Simulations: Materials Design and Discovery,

  Berlin, Germany, Feb. 1 - 5, 2015.

- *High-throughput Screening of Perovskite Oxides and Related Compounds for Light harvesting Applications*

  DPG Spring Meeting,

  Berlin, Germany, Mar. 15 - 20, 2015.

- *High-Throughput Computational Screening of Rare-Earth Perovskite Oxides for Light Harvesting Applications*

  PASC15,

Zürich, Switzerland, Jun. 1 - 3, 2015.

- *Novel Light Harvesting Materials*

  MARVEL Junior Retreat,

  Männedorf, Switzerland, Jul. 7 - 10, 2015.

- *Validation and Verification of Pseudopotentials: the Standard Solid State Pseudopotential (SSSP) Library*

  Ψ_K 2015 Conference,

  San Sebastian, Spain, Sep. 6 - 10, 2015.

- *First Principle Study of the Electrochemical Interface of Ethyl Methyl Carbonate and LP57*

  Liquid/Solid Interfaces: Structure and Dynamics from Spectroscopy and Simulations - 3rd Edition,

  CECAM-HQ-EPFL, Lausanne, Switzerland, Jan 25 - 27, 2016.

Teaching and Supervision Experience

- Teaching Assistance:
  - *Advanced Quantum Mechanics*, master degree in Physics (10 ECTS) - DTU, Fall 2010 and Fall 2011.
  - *Quantum Mechanics*, bachelor degree in Physics (10 ECTS) - DTU, Spring 2011.
  - *Electronic Structure Methods in Material Physics, Chemistry and Biology*, master degree in Physics (10 ECTS) - DTU, Spring 2014.
  - *Physique Générale III* and *IV*, bachelor degree in Physics (6 and 4 ECTS) - EPFL, Fall 2014 and Spring 2015.
  - *Quantum simulations of materials: Properties and spectroscopies*, master degree in Physics (4 ECTS) - EPFL, Fall 2014.
- Lectures in Courses:
  - *Sustainable Chemistry*, master degree in Chemistry (15 ECTS) - University of Copenhagen, Spring 2016 and Spring 2017.
  - *Battery Materials and Chemistries: from Fundamental Mechanisms to Battery Cells*, master course (5 ECTS) - DTU, Fall 2017.
  - *Advanced Computational Tools for Energy Materials*, master course (5 ECTS) - DTU, Fall 2017.
- Special Courses (5 ECTS):
  - Daniel Christoffer Nielsen (master student), *Calculation of Absorption Spectra Using Time-Dependent Density Functional Theory* - DTU, January 2012.
  - Kåre W. Jacobsen (master student), *Data Mining in Perovskites* - DTU, Spring 2014.
  - Vasileios Bilalis (master student), *Photoferroic Materials for Electrocatalytic Reactions* - DTU, Fall 2017.
- Co-supervised Ph.D. students:
  - Felix Tim Bölle, *Machine Learning and Ab-initio Simulations for Accelerated Materials Discovery*, 2018, Feb - 2021, Jan.
- Co-supervised research assistants:

  - August Edwards Guldberg Mikkelsen, 2018, Feb - Aug.

- Co-supervised bachelor and master students:
  - Mathias Dam Spo, *Trends in Adsoprtion Energy on p− and n−type TiO_2*, bachelor degree in Chemistry - University of Copenhagen, Spring 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*, master degree in Chemistry - University of Copenhagen, Fall 2015 - Spring 2016.

Administrative and Organizative Experience

- Member of *MX Library Committee*, EPFL, 2014, Nov. - 2015, Aug.
- Organizer of *MARVEL Junior Retreat*, Hotel Boldern, Männedorf, Switzerland, Jul. 7 - 10, 2015.
- Member of *Junior Investigator Network 2016* and *Junior Investigator Alumni*, Copenhagen University.
- Referee for the following journals: Applied Surface Science, Chemical Science, Chemistry of Materials, Journal of Physical Chemistry C and Letters, Scientific Data, Nanotechnology, 2D Materials, Topics in Catalysis, ChemPhysChem, ChemSusChem, Journal of Physics D: Applied Physics, npj Computational Materials, Chemistry - A European Journal.

Languages

Italian, English, French, Danish.

Computing

- Environments: unix (linux), Windows.
- Programming: c/c++, Mathematica, perl, python, fortran, unix shell/awk, matplotlib, html.
- Editors/utilities: emacs, latex, xmgrace, gimp, MS/open office.
- Ab-initio codes and environments: GPAW, ASE, QUANTUM Espresso, AiiDA, VNL/ATK, QM^{4}D, VASP.

Last updated: March 7, 2018