Annex 1 Publication list

All publications have been entered in NIRA, and are listed below, sorted by group leaders. We list publications either resulting directly from the NCCR (marked with a red hexagon) or with minor contributions from the NCCR. The following lists cover the period from May 1st, 2014 to January 31st, 2017.

1. Scientific articles in journals with peer review
2. Scientific articles in journals without peer review
3. Publications from lists 1 and 2 involving several groups

1. Scientific articles in journals with peer review

Group of Wanda Andreoni

- C. Ma, F. Pietrucci, and W. Andreoni
  Reaction dynamics of CO_2 in aqueous amines from ab initio molecular dynamics: 2-amino-2-methyl-1,3-propanediol (AMPD) compared to monoethanolamine (MEA)
  Theoretical Chemistry Accounts **135**, 60 (2016).
  Group(s): Andreoni / Project(s): VP2

W. Andreoni and F. Pietrucci
CO_2 capture in amine solutions: modelling and simulations with non-empirical methods
Journal of Physics: Condensed Matter **28**, 503003 (2016).
Group(s): Andreoni / Project(s): VP2

Group of Claudia Cancellieri

- F. Evangelisti, M. Stiefel, O. Guseva, R. P. Nia, R. Hauert, E. Hack, L. P. H. Jeurgens, F. Ambrosio, A. Pasquarello, P. Schmutz, and C. Cancellieri
  Electronic and structural characterization of barrier-type amorphous aluminium oxide
  Electrochimica Acta **224**, 503 (2017).
  Group(s): Cancellieri, Pasquarello / Project(s): VP2, PP7

Group of Michele Ceriotti

- S. De, F. Musil, T. Ingram, C. Baldauf, and M. Ceriotti
  Mapping and classifying molecules from a high-throughput structural database
  Journal of Cheminformatics **9**, 6 (2017).
  Group(s): Ceriotti / Project(s): HP5

- S. De, A. P. Bartók, G. Csányi, and M. Ceriotti
  Comparing molecules and solids across structural and alchemical space
  Physical Chemistry Chemical Physics **18**, 13754 (2016).
  Group(s): Ceriotti / Project(s): HP5

M. Rossi, P. Gasparotto, and M. Ceriotti
Anharmonic and Quantum Fluctuations in Molecular Crystals: A First-Principles Study of the Stability of Paracetamol
Physical Review Letters **117**, 115702 (2016).
Group(s): Ceriotti / Project(s): HP4

P. Gasparotto, A. A. Hassanali, and M. Ceriotti
Probing Defects and Correlations in the Hydrogen-Bond Network of ab Initio Water
Journal of Chemical Theory and Computation **12**, 1953 (2016).
Group(s): Ceriotti / Project(s): HP4

- V. Kapil, J. VandeVondele, and M. Ceriotti

Accurate molecular dynamics and nuclear quantum effects at low cost by multiple steps in real and imaginary time: Using density functional theory to accelerate wavefunction methods

The Journal of Chemical Physics **144**, 054111 (2016).

Group(s): Ceriotti, VandeVondele / Project(s): HP3,HP4

R. Petraglia, A. Nicolaï, M. D. Wodrich, M. Ceriotti, and C. Corminboeuf

Beyond Static Structures: Putting Forth REMD as a Tool to Solve Problems in Computational Organic Chemistry

Journal of Computational Chemistry **37**, 83 (2016).

Group(s): Ceriotti, Corminboeuf / Project(s): HP4

A. Ardevol, G. A. Tribello, M. Ceriotti, and M. Parrinello

Probing the Unfolded Configurations of a β-Hairpin Using Sketch-Map

Journal of Chemical Theory and Computation **11**, 1086 (2015).

Group(s): Ceriotti, Parrinello / Project(s): HP4

- P. Gasparotto and M. Ceriotti

Recognizing molecular patterns by machine learning: An agnostic structural definition of the hydrogen bond

The Journal of Chemical Physics **141**, 174110 (2014).

Group(s): Ceriotti / Project(s): HP4

Group of Volkan Cevher

- D. Carlson, Y.-P. Hsieh, E. Collins, L. Carin, and V. Cevher

Stochastic Spectral Descent for Discrete Graphical Models

IEEE Journal of Selected Topics in Signal Processing (2016), doi:10.1109/JSTSP.2015.2505684.

Group(s): Cevher, Koch / Project(s): HP5

A. Norouzi-Fard, A. Bazzi, I. Bogunovic, M. El Halabi, Y.-P. Hsieh, and V. Cevher

An Efficient Streaming Algorithm for the Submodular Cover Problem

in *Advances in Neural Information Processing Systems 29 (NIPS 2016)*, D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett., eds. (2016).

Group(s): Cevher / Project(s): HP5

- D. E. Carlson, E. Collins, Y.-P. Hsieh, L. Carin, and V. Cevher

Preconditioned Spectral Descent for Deep Learning

in *Advances in Neural Information Processing Systems 28 (NIPS 2015)*, C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett, eds. (2015).

Group(s): Cevher, Koch / Project(s): HP5

Group of Clémence Corminboeuf

- M. Wodrich, M. Busch, and C. Corminboeuf

Accessing and predicting the kinetic profiles of homogeneous catalysts from volcano plots

Chemical Science **7**, 5723 (2016).

Group(s): Corminboeuf / Project(s): VP2

R. Petraglia, A. Nicolaï, M. D. Wodrich, M. Ceriotti, and C. Corminboeuf

Beyond Static Structures: Putting Forth REMD as a Tool to Solve Problems in Computational Organic Chemistry

Journal of Computational Chemistry **37**, 83 (2016).

Group(s): Ceriotti, Corminboeuf / Project(s): HP4

- M. Busch, M. Wodrich, and C. Corminboeuf

Linear Scaling Relationships and Volcano Plots in Homogeneous Catalysis ? Revisiting the Suzuki Reaction

Chemical Science **6**, 6754 (2015).

Group(s): Corminboeuf / Project(s): VP2

- G. Gryn'ova, M. Coote, and C. Corminboeuf

Theory and practice of uncommon molecular electronic configurations

WIREs Computational Molecular Science **5**, 440 (2015).

Group(s): Corminboeuf / Project(s): VP2

Group of Alessandro Curioni

P. Staar, M. Jiang, U. R. Hähner, T. C. Schulthess, and T. A. Maier

Interlaced coarse-graining for the dynamic cluster approximation

Physical Review B **93**, 165144 (2016).

Group(s): Curioni, Schulthess / Project(s): HP5

P. W. J. Staar, P. K. Barkoutsos, R. Istrate, A. C. I. Malossi, I. Tavernelli, N. Moll, H. Giefers, C. Hagleitner, C. Bekas, and A. Curioni

Stochastic matrix-function estimators: Scalable Big-Data kernels with high performance

in *2016 IEEE International Parallel and Distributed Processing Symposium (IPDPS)* (2016),

p. 812, doi:10.1109/IPDPS.2016.34.
Group(s): Curioni / Project(s): HP5

F. Franco de Carvalho and I. Tavernelli
Nonadiabatic dynamics with intersystem crossings: A time-dependent density functional theory implementation
The Journal of Chemical Physics **143**, 224105 (2015).
Group(s): Curioni / Project(s): VP2

- K. Meier, T. Laino, and A. Curioni
Solid-State Electrolytes: Revealing the Mechanisms of Li-Ion Conduction in Tetragonal and Cubic LLZO by First-Principles Calculations
The Journal of Physical Chemistry C **118**, 6668 (2014).
Group(s): Curioni / Project(s): VP2

Group of Antoine Georges

M. Kim, Y. Nomura, M. Ferrero, P. Seth, O. Parcollet, and A. Georges
Enhancing superconductivity in A_3C_{60} fullerides
Physical Review B **94**, 155152 (2016).
Group(s): Georges / Project(s): VP1

J. Mravlje and A. Georges
Thermopower and Entropy: Lessons from Sr_2RuO_4
Physical Review Letters **117**, 036401 (2016).
Group(s): Georges / Project(s): VP1

- M. Aichhorn, L. Pourovskii, P. Seth, V. Vildosola, M. Zingl, O. E. Peil, X. Deng, J. Mravlje, G. J. Kraberger, C. Martins, M. Ferrero, and O. Parcollet
TRIQS/DFTTools: A TRIQS application for ab initio calculations of correlated materials
Computer Physics Communications **204**, 200 (2016).
Group(s): Georges / Project(s): VP1

H. T. Dang, J. Mravlje, A. Georges, and A. J. Millis
Band Structure and Terahertz Optical Conductivity of Transition Metal Oxides: Theory and Application to $CaRuO_3$
Physical Review Letters **115**, 107003 (2015).
Group(s): Georges / Project(s): VP1

H. T. Dang, J. Mravlje, A. Georges, and A. J. Millis
Electronic correlations, magnetism, and Hund's rule coupling in the ruthenium perovskites $SrRuO_3$ and $CaRuO_3$
Physical Review B **91**, 195149 (2015).
Group(s): Georges / Project(s): VP1

- A. Subedi, O. E. Peil, and A. Georges
Low-energy description of the metal-insulator transition in the rare-earth nickelates
Physical Review B **91**, 075128 (2015).
Group(s): Georges / Project(s): VP1

- J. Ruppen, J. Teyssier, O. E. Peil, S. Catalano, M. Gibert, J. Mravlje, J.-M. Triscone, A. Georges, and D. van der Marel
Optical spectroscopy and the nature of the insulating state of rare-earth nickelates
Physical Review B **92**, 155145 (2015).
Group(s): Georges, van der Marel / Project(s): VP1, PP7

D. Stricker, J. Mravlje, C. Berthod, R. Fittipaldi, A. Vecchione, A. Georges, and D. van der Marel
Optical Response of Sr_2RuO_4 Reveals Universal Fermi-Liquid Scaling and Quasiparticles Beyond Landau Theory
Physical Review Letters **113**, 087404 (2014).
Group(s): Georges / Project(s): VP1

O. E. Peil, M. Ferrero, and A. Georges
Orbital polarization in strained $LaNiO_3$: Structural distortions and correlation effects
Physical Review B **90**, 045128 (2014).
Group(s): Georges / Project(s): VP1

Group of Stefan Goedecker

- G. Fisicaro, L. Genovese, O. Andreussi, N. Marzari, and S. Goedecker
A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments
The Journal of Chemical Physics **144**, 014103 (2016).
Group(s): Goedecker, Marzari / Project(s): HP3

- L. Zhu, M. Amsler, T. Fuhrer, B. Schaefer, S. Faraji, S. Rostami, S. A. Ghasemi, A. Sadeghi, M. Grauzinyte, C. Wolverton, and S. Goedecker
A fingerprint based metric for measuring similarities of crystalline structures
The Journal of Chemical Physics **144**, 034203 (2016).
Group(s): Goedecker / Project(s): HP4

- B. Schaefer and S. Goedecker
Computationally efficient characterization of potential energy surfaces based on fingerprint distances
The Journal of Chemical Physics **145**, 034101

(2016).

Group(s): Goedecker / Project(s): HP4

- J. A. Flores-Livas, M. Amsler, C. Heil, A. Sanna, L. Boeri, G. Profeta, C. Wolverton, S. Goedecker, and E. K. U. Gross
  Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure
  Physical Review B **93**, 020508 (2016).
  Group(s): Goedecker / Project(s): HP4

- 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. Dulak, 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 (2016).
  Group(s): Goedecker, Marzari / Project(s): PP6, VP2

M. Amsler, S. Botti, M. A. L. Marques, T. J. Lenosky, and S. Goedecker
Low-density silicon allotropes for photovoltaic applications
Physical Review B **92**, 014101 (2015).
Group(s): Goedecker / Project(s): HP4

B. Schaefer, S. A. Ghasemi, S. Roy, and S. Goedecker
Stabilized quasi-Newton optimization of noisy potential energy surfaces
The Journal of Chemical Physics **142**, 034112 (2015).
Group(s): Goedecker / Project(s): HP4

Group of Jürg Hutter

F. H. Hodel and S. Luber
Redox-Inert Cations Enhancing Water Oxidation Activity: The Crucial Role of Flexibility
ACS Catalysis **6**, 6750 (2016).
Group(s): Hutter / Project(s): VP2

F. H. Hodel and S. Luber
What Influences the Water Oxidation Activity of a Bioinspired Molecular $Co_4^{II}O_4$ Cubane? An In-Depth Exploration of Catalytic Pathways
ACS Catalysis **6**, 1505 (2016).
Group(s): Hutter / Project(s): VP2

M. Schilling, G. R. Patzke, J. Hutter, and S. Luber
Computational Investigation and Design of Cobalt Aqua Complexes for Homogeneous Water Oxidation
The Journal of Physical Chemistry C **120**, 7966 (2016).
Group(s): Hutter / Project(s): VP2

G. Mette, D. Sutter, Y. Gurdal, S. Schnidrig, B. Probst, M. Iannuzzi, J. Hutter, R. Alberto, and J. Osterwalder
From porphyrins to pyrphyrins: adsorption study and metalation of a molecular catalyst on Au(111)
Nanoscale **8**, 7958 (2016).
Group(s): Hutter / Project(s): VP2

- G. Miceli, J. Hutter, and A. Pasquarello
  Liquid Water through Density-Functional Molecular Dynamics: Plane-Wave vs Atomic-Orbital Basis Sets
  Journal of Chemical Theory and Computation **12**, 3456 (2016).
  Group(s): Hutter, Pasquarello / Project(s): VP2,HP3

- J. Wilhelm, M. Del Ben, and J. Hutter
  GW in the Gaussian and Plane Waves Scheme with Application to Linear Acenes
  Journal of Chemical Theory and Computation **12**, 3623 (2016).
  Group(s): Hutter / Project(s): HP3

- J. Wilhelm, P. Seewald, M. Del Ben, and J. Hutter
  Large-Scale Cubic-Scaling Random Phase Approximation Correlation Energy Calculations Using a Gaussian Basis
  Journal of Chemical Theory and Computation **12**, 5851 (2016).
  Group(s): Hutter / Project(s): HP3

F. Evangelisti, R. Moré, F. Hodel, S. Luber, and G. R. Patzke

3d–4f $Co^{II}_3Ln(OR)_4$ Cubanes as Bio-Inspired Water Oxidation Catalysts

Journal of the American Chemical Society **137**, 11076 (2015).

Group(s): Hutter / Project(s): VP2

- Y. Gurdal, S. Luber, J. Hutter, and M. Iannuzzi
  Non-innocent adsorption of Co-pyrphyrin on rutile(110)

  Physical Chemistry Chemical Physics **17**, 22846 (2015).

  Group(s): Hutter / Project(s): VP2

- M. Del Ben, O. Schütt, T. Wentz, P. Messmer, J. Hutter, and J. VandeVondele
  Enabling simulation at the fifth rung of DFT: Large scale RPA calculations with excellent time to solution

  Computer Physics Communications **187**, 120 (2015).

  Group(s): Hutter, VandeVondele / Project(s): HP3

- M. Del Ben, J. Hutter, and J. VandeVondele
  Forces and stress in second order Møller-Plesset perturbation theory for condensed phase systems within the resolution-of-identity Gaussian and plane waves approach

  The Journal of Chemical Physics **143**, 102803 (2015).

  Group(s): Hutter, VandeVondele / Project(s): HP3

- M. Del Ben, J. Hutter, and J. VandeVondele
  Probing the structural and dynamical properties of liquid water with models including non-local electron correlation

  The Journal of Chemical Physics **143**, 054506 (2015).

  Group(s): Hutter, VandeVondele / Project(s): HP3

U. Borštnik, J. VandeVondele, V. Weber, and J. Hutter
Sparse matrix multiplication: The distributed block-compressed sparse row library

Parallel Computing **40**, 47 (2014).

Group(s): Hutter, VandeVondele / Project(s): HP3

Group of Christoph Koch

- A. Shaikhha, Y. Klonatos, L. Parreaux, L. Brown, M. Dashti, and C. Koch
  How to Architect a Query Compiler

  in *Proceedings of the 2016 International Conference on Management of Data* (ACM, New York, NY, USA, 2016), SIGMOD '16, p. 1907.

  Group(s): Koch / Project(s): HP5

I. Trummer and C. Koch
Multiple Query Optimization on the D-Wave 2X Adiabatic Quantum Computer

Proceedings of the VLDB Endowment **9**, 660 (2016), arXiv:1510.06437.

Group(s): Koch / Project(s): HP5

- D. Carlson, Y.-P. Hsieh, E. Collins, L. Carin, and V. Cevher
  Stochastic Spectral Descent for Discrete Graphical Models

  IEEE Journal of Selected Topics in Signal Processing (2016), doi:10.1109/JSTSP.2015.2505684.

  Group(s): Cevher, Koch / Project(s): HP5

- D. E. Carlson, E. Collins, Y.-P. Hsieh, L. Carin, and V. Cevher
  Preconditioned Spectral Descent for Deep Learning

  in *Advances in Neural Information Processing Systems 28 (NIPS 2015)*, C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett, eds. (2015).

  Group(s): Cevher, Koch / Project(s): HP5

Group of Thomas Lippert

- W. Si, D. Pergolesi, F. Haydous, A. Fluri, A. Wokaun, and T. Lippert
  Investigating the behavior of various cocatalysts on $LaTaON_2$ photoanode for visible light water splitting

  Physical Chemistry Chemical Physics **19**, 656 (2017).

  Group(s): Lippert, Pergolesi / Project(s): PP7

Group of Nicola Marzari

Y. Hinuma, G. Pizzi, Y. Kumagai, F. Oba, and I. Tanaka
Band structure diagram paths based on crystallography

Computational Materials Science **128**, 140 (2017).

Group(s): Marzari / Project(s): PP6

- N. Marzari
  Materials modelling: The frontiers and the challenges

  Nature Materials **15**, 381 (2016).

  Group(s): Marzari / Project(s): VP2

- G. Pizzi, M. Gibertini, E. Dib, N. Marzari, G. Iannaccone, and G. Fiori
  Performance of arsenene and antimonene double-gate MOSFETs from first principles

Nature Communications **7**, 12585 (2016).
Group(s): Marzari / Project(s): VP2

T. Y. Kim, C.-H. Park, and N. Marzari
The Electronic Thermal Conductivity of Graphene
Nano Letters **16**, 2439 (2016).
Group(s): Marzari / Project(s): VP2

A. Cepellotti and N. Marzari
Thermal Transport in Crystals as a Kinetic Theory of Relaxons
Physical Review X **6**, 041013 (2016).
Group(s): Marzari / Project(s): VP2

J. Hu, G. M. Vanacore, A. Cepellotti, N. Marzari, and A. H. Zewail
Rippling ultrafast dynamics of suspended 2D monolayers, graphene
Proceedings of the National Academy of Science of the USA **113**, E6555 (2016).
Group(s): Marzari / Project(s): VP2

G. Fisicaro, L. Genovese, O. Andreussi, N. Marzari, and S. Goedecker
A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments
The Journal of Chemical Physics **144**, 014103 (2016).
Group(s): Goedecker, Marzari / Project(s): HP3

N. L. Nguyen, G. Borghi, A. Ferretti, and N. Marzari
First-Principles Photoemission Spectroscopy of DNA and RNA Nucleobases from Koopmans-Compliant Functionals
Journal of Chemical Theory and Computation **12**, 3948 (2016).
Group(s): Marzari / Project(s): HP3

M. M. Montemore, O. Andreussi, and J. W. Medlin
Hydrocarbon adsorption in an aqueous environment: A computational study of alkyls on Cu(111)
The Journal of Chemical Physics **145**, 074702 (2016).
Group(s): Marzari / Project(s): HP4

L. Sementa, O. Andreussi, W. A. Goddard, and A. Fortunelli
Catalytic activity of Pt_{38} in the oxygen reduction reaction from first-principles simulations
Catalysis Science & Technology **6**, 6901 (2016).
Group(s): Marzari / Project(s): HP4

G. W. Mann, K. Lee, M. Cococcioni, B. Smit, and J. B. Neaton
First-principles Hubbard U approach for small molecule binding in metal-organic frameworks
The Journal of Chemical Physics **144**, 174104 (2016).
Group(s): Marzari, Smit / Project(s): HP4

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. Dulak, 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 (2016).
Group(s): Goedecker, Marzari / Project(s): PP6, VP2

G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, and B. Kozinsky
AiiDA: automated interactive infrastructure and database for computational science
Computational Materials Science **111**, 218 (2016).
Group(s): Marzari / Project(s): PP6

M. Gibertini and N. Marzari
Emergence of One-Dimensional Wires of Free Carriers in Transition-Metal-Dichalcogenide Nanostructures
Nano Letters **15**, 6229 (2015).
Group(s): Marzari / Project(s): VP2, VP1

Y. Krupskaya, M. Gibertini, N. Marzari, and A. F. Morpurgo
Band-Like Electron Transport with Record-High Mobility in the TCNQ Family
Advanced Materials **27**, 2453 (2015).
Group(s): Marzari / Project(s): VP2

D. Dumcenco, D. Ovchinnikov, K. Marinov, P. Lazić, M. Gibertini, N. Marzari, O. L. Sanchez, Y.-C. Kung, D. Krasnozhon, M.-W. Chen, S. Bertolazzi,

P. Gillet, A. Fontcuberta i Morral, A. Radenovic, and A. Kis
Large-Area Epitaxial Mono layer MoS_2
ACS Nano **9**, 4611 (2015).
Group(s): Marzari / Project(s): VP2

A. Cepellotti, G. Fugallo, L. Paulatto, M. Lazzeri, F. Mauri, and N. Marzari
Phonon hydrodynamics in two-dimensional materials
Nature Communications **6**, 6400 (2015).
Group(s): Marzari / Project(s): VP2

D. Dragoni, D. Ceresoli, and N. Marzari
Thermoelastic properties of α-iron from first-principles
Physical Review B **91**, 104105 (2015).
Group(s): Marzari / Project(s): VP2

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
Chemistry of Materials **27**, 7662 (2015).
Group(s): Marzari, Schmidt / Project(s): PP7, VP2

I. Timrov, O. Andreussi, A. Biancardi, N. Marzari, and S. Baroni
Self-consistent continuum solvation for optical absorption of complex molecular systems in solution
The Journal of Chemical Physics **142**, 034111 (2015).
Group(s): Marzari / Project(s): HP3

X. Qian, P. Umari, and N. Marzari
First-principles investigation of organic photovoltaic materials C_{60}, C_{70}, $[C_{60}]$PCBM, and bis-$[C_{60}]$PCBM using a many-body G_0W_0-Lanczos approach
Physical Review B **91**, 245105 (2015).
Group(s): Marzari / Project(s): HP3

N. L. Nguyen, G. Borghi, A. Ferretti, I. Dabo, and N. Marzari
First-Principles Photoemission Spectroscopy and Orbital Tomography in Molecules from Koopmans-Compliant Functionals
Physical Review Letters **114**, 166405 (2015).
Group(s): Marzari / Project(s): HP3

G. Borghi, C.-H. Park, N. L. Nguyen, A. Ferretti, and N. Marzari
Variational minimization of orbital-density-dependent functionals
Physical Review B **91**, 155112 (2015).
Group(s): Marzari / Project(s): HP3

N. Bonnet, I. Dabo, and N. Marzari
Chemisorbed Molecules under Potential Bias: Detailed Insights from First-Principles Vibrational Spectroscopies
Electrochimica Acta **121**, 210 (2014).
Group(s): Marzari / Project(s): VP2

O. Andreussi and N. Marzari
Electrostatics of solvated systems in periodic boundary conditions
Physical Review B **90**, 245101 (2014).
Group(s): Marzari / Project(s): VP2

M. Gibertini, G. Pizzi, and N. Marzari
Engineering polar discontinuities in honeycomb lattices
Nature Communications **5**, 5157 (2014).
Group(s): Marzari / Project(s): VP2

M. Gibertini, F. M. D. Pellegrino, N. Marzari, and M. Polini
Spin-resolved optical conductivity of two-dimensional group-VIB transition-metal dichalcogenides
Physical Review B **90**, 245411 (2014).
Group(s): Marzari / Project(s): VP2

N. Bonnet and N. Marzari
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3. Publications involving several groups

Publications with peer review

- F. Evangelisti, M. Stiefel, O. Guseva, R. P. Nia, R. Hauert, E. Hack, L. P. H. Jeurgens, F. Ambrosio, A. Pasquarello, P. Schmutz, and C. Cancellieri
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  Group(s): Troyer, Yazyev / Project(s): VP1

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- G. Fisicaro, L. Genovese, O. Andreussi, N. Marzari, and S. Goedecker
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Group(s): Hutter, VandeVondele / Project(s): HP3

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Group(s): Ceriotti, Parrinello / Project(s): HP4

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Group(s): Hutter, VandeVondele / Project(s): HP3

Submitted publications

- 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

  submitted (2016).

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N. Xu, G. Autès, C. E. Matt, B. Q. Lv, M. Y. Yao, F. Bisti, V. N. Strocov, D. Gawryluk, E. Pomjakushina, K. Conder, N. C. Plumb, M. Radovic, T. Qian, O. V. Yazyev, J. Mesot, H. Ding, and M. Shi
Distinct evolutions of Weyl fermion quasiparticles and Fermi arcs with bulk band topology in Weyl semimetals
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