Simone Piccinin

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Career Summary

Senior Researcher (*primo ricercatore*)	Mar. 2020 – present	CNR-IOM - Trieste
Researcher (*permanent*)	Nov. 2011 – Feb 2020	CNR-IOM - Trieste
Researcher (*fixed term*)	May 2009 – Nov. 2011	CNR-IOM - Trieste
Postdoc	Dec. 2008 – May 2009	SISSA - Trieste Condensed Matter Sector Supervisor: Prof. Stefano Baroni
Postdoc	Nov 2006 – Dec. 2008	University of Sydney School of Physics Supervisor: Prof. Catherine Stampfl
Postdoc	Sept. 2006 – Oct. 2006	Princeton University Dept. of Chemistry Supervisor: Prof. Roberto Car

Education

Ph.D. in Chemistry	Sept. 2006	Princeton University Thesis: *Theoretical modeling of electronic transport in molecular devices* Supervisor: Prof. Roberto Car
Laurea (M.S.) in Materials Eng. (summa cum laude)	July 2001	University of Trieste Thesis: *Adsorption and diffusion of Co adatoms on Ag(111)* Supervisor: Prof. Alessandro De Vita

Awards

- Marie Curie Fellowship, 2009-2013
- Hugh Stott Taylor Fellowship, awarded by Princeton University, 2001-2005
- Graduate School Fellowship, awarded by Princeton University, 2001-2006
- Habilitation to Associate Professor in condensed matter physics, physical chemistry, inorganic chemistry (*Abilitazione Scientifica Nazionale* in S.S.D. 02/B2, 03/A2, 03/B1)

Research Grants

- EU H2020-INFRAIA-2014/2015, EUR 10,000,000, Funding period: 2015-2019
  Title: *Nanoscience foundries and fine analysis for Europe*
  Role: participant (PI: Prof. Giorgio Rossi)
- Marie Curie IRG grant (FP7-PEOPLE-IRG-2008), EUR 100,000, Funding period: 2009-2013
  Title: *Water splitting catalysts for artificial photosynthesis.*
  Role: Marie Curie Fellow

- Young SISSA Scientists' Research Projects, EUR 6,500, Funding period: 2011-2012
  Title: *Water splitting catalysts for artificial photosynthesis*
  Role: PI
- ARC Discovery Project (DP0984389), AU$ 370,000, Funding period: 2009-2011
  Title: *First-Principles Engineering of Advanced Multicomponent Materials for Clean, Energy Efficient Thermoelectric and Catalytic Technologies*
  Role: co-PI (PI: Prof. Catherine Stampfl)
- PRIN 2010-2011, EUR 1,565,550, Funding period: 2013-2016
  Title: *Frontiere della ricerca sul grafene: comprensione e controllo di funzionalità avanzate*
  Role: participant (PI: Prof. Alberto Morgante)

Computational Grants (as Principal Investigator)

- ISCRA 2020/2021 Type B (1.5 million CPU hours), *Controlling the oxidizability of supported Platinum nanoclusters*
- ISCRA 2018/2019 Type B (3.5 million CPU hours), *Thin Iridium oxide-like layers as model catalysts for water oxidation*
- PRACE 2016/2017 (28.0 million CPU hours), *Modelling proton-coupled electron transfers in water oxidation on hematite*
- ISCRA 2016/2017 Type B (2.2 million CPU hours), *Energy level alignment in p-type DSSCs: Modeling organic dye adsorption on NiO(100)*
- ISCRA 2015/2016 Type C (200,000 CPU hours), *Direct role of molecular oxygen in oxidation reactions*
- PRACE 2014/2015 (11.0 million CPU hours), *Kinetic modeling of ethylene epoxidation on Ag surfaces*
- ISCRA 2014/2015 Type B (3.1 million CPU hours), *First-principles assessment of CO2 activation over metal surfaces*
- PRACE 2012/2013 (12.0 million CPU hours), *Engineering multi-core transition metal catalysts for solar fuel production*
- ISCRA 2012/2013 Type B (4.6 million CPU hours), *First-principles investigation of supported Au clusters for heterogeneous catalysis*
- PRACE 2011/2012 (4.8 million CPU hours), *Multicenter cobalt-oxo cores for catalytic water oxidation*
- ISCRA 2011/2012 Type B (165,000 CPU hours), *The Role of Sub-surface Oxygen in Ethylene Epoxidation on Ag-Cu alloys*
- PRACE Preparatory Access 2011 (50,000 CPU hours), *Water splitting catalysts for artificial photosynthesis*
- DEISA/DECI 2010/2011 (1.5 million CPU hours), *Water splitting catalysts for artificial photosynthesis*

Travel Grants

- CNR Short Term Mobility Grant, 2016
- CNR Short Term Mobility Grant, 2013
- ARNAM (Australian Research Network for Advanced Materials) Grant, 2008

Teaching Experience

Lecturer at CECAM electronic structure summer schools	Jun.-Jul. 2011, 2012, 2013, 2014	SISSA, Trieste
Lecturer at School on computational materials modeling in catalysis	1-5 Sept 2014	JNCASR, Bangalore
Lecturer at Quantum ESPRESSO summer school	8-12 Jul 2013	Fudan University, Shanghai

Lecturer at Quantum ESPRESSO summer school	29 Nov – 2 Dec 2010	JNCASR, Bangalore
Teaching assistant for the General Chemistry Laboratory	Sept 2002 – May 2006 (3 semesters, full time)	Princeton University Department of Chemistry

Supervising Experience

Supervisor or co-supervisor of the following students/postdocs:

Masters Students

- Luca Dietz, Politecnico di Milano, Department of Chemistry, Materials and Chemical Engineering, *First-principles assessment of CO_2 activation over metal surfaces* (2013)

Ph.D. Students

- Xuejun Gong, SISSA Condensed Matter, 2020 - present
- Mina Taleblou, University of Trieste, School of Nanotechnology, 2019 - present
- Matteo Ferri, SISSA Condensed Matter, *Ab-initio Characterization of a Novel Photocathode for Water Splitting: Bulk and Surface Properties of $CuFeO_2$*, 2016 - 2020
- Changru Ma, SISSA Condensed Matter, *Modeling Ru-based molecular catalysts for water oxidation,* 2009-2012
- Linh Ngoc Nguyen, SISSA Condensed Matter, *Toward Realistic DFT Description of Complex Systems: Ethylene Epoxidation on Ag-Cu Alloys and RPA Correlation in van der Waals Molecules,* 2009-2012

Postdocs

- Giulia Righi, PhD. University of Modena and Reggio Emilia (Italy), 11/2019 – present
- Fatema Mohamed, Ph.D. University of Trieste (Italy), 07/2019 – 07/2020
- Travis Jones, Ph.D. Colorado School of Mines (USA), 05/2012 – 07/2014
- Karolina Kwapien, Ph.D. Humboldt University (Germany), 07/2012 – 07/2014
- Praveen Chandramathy Surendran, Ph.D. University of Nova Goriza (Slovenia), 09/2012 – 09/2014

Scientific Visits

Fritz-Haber-Institute, Berlin	Nov. 2016 – Dec. 2016	Host: Prof. Robert Schlögl
Yonsei University	Nov. 2014	Host: Prof. Aloysius Soon
University College London	June 2013 – July 2013	Host: Dr. Michail Stamatakis
Univ. of Sydney	Nov. 2011 – Dec. 2011	Host: Prof. Catherine Stampfl
JNCASR, Bangalore	Nov. 2010	Host: Prof. Shobhana Nasasimhan
Keio University, Tokyo	Apr. 2008	Host: Prof. Hiroshi Kondoh
King's College, London	Jan. 2008	Host: Prof. Alessandro De Vita
Fritz-Haber-Institute, Berlin	Dec. 2007	Host: Prof. Matthias Scheffler
ICTP, Trieste	July 2003 – Sept. 2003	Host: Prof. Ralph Gebauer

Organization of scientific meetings

- Organizer of the ICTP workshop “Workshop on physics and chemistry of solid/liquid interfaces for energy conversion and storage”, Trieste (Italy), 25-29 May, 2020.

- Organizer of the CECAM/Psi-K workshop “Interface processes in photochemical water splitting: Theory meets experiment”, Lausanne (Switzerland), 27-30 September 2016.
- Organizer of the Shell-CECAM workshop "From the chemical bond to the chemical reactor: Computational and Materials challenges in gas conversion technologies", Bangalore (India), Aug. 25-29, 2014.
- Organizer of the “CECAM Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology and Biophysics” at SISSA, Trieste (Italy), 30 June-18 July 2014
- Organizer of the “Joint ICTP-NSFC School and Advanced Workshop on Modern Electronic Structure Computations”, Shanghai (China), 8-12 July 2013
- Organizer of the “CECAM Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology and Biophysics” at SISSA, Trieste (Italy), 8-26 July 2013
- Organizer of the “CECAM Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology and Biophysics” at SISSA, Trieste (Italy), 9-28 July 2012

Other professional activities

- Associate Editor - Journal of Materials for Renewable and Sustainable Energy - Springer Ed. (2019-present).
- Evaluator for scientific projects for the following agencies: ERC (EU), PRACE (EU), Polish National Science Centre (Poland), ACS Petroleum Research Fund, Cineca (Italy).
- Reviewer for the following scientific journals: ACS Catalysis, J. Chem. Phys., J. Phys. Chem., PCCP, Phys. Rev. B, Surface Science.
- Director of the Quantum Espresso Foundation, Feb 2012 – Aug. 2013 (http://foundation.quantum-espresso.org/)

Invited Talks at Conferences and Workshops

- FISMAT 2019, University of Catania (Italy), 30 September - 4 October 2019, *Theoretical modeling of Fe2O3 electrodes for photocatalytic water oxidation.*
- Workshop “Structure-dependent microkinetic analysis: theory and experiments”, Monteisola (Italy), 13-15 June 2018, *The selective oxygen species in ethylene epoxidation on silver: Insights from DFT simulations and in situ experiments.*
- International Conference on Electronic Materials and Nanotechnology for Green Environment 2016 (ENGE2016), Jeju (South Korea), November 6-9 (2016), *The Electronic Structure of the Oxygen Species Active in Ethylene Epoxidation on Ag.*
- ICTP "Workshop on Materials Science for Energy Storage", Trieste (Italy), 11-15 May 2015, *DFT modeling of water oxidation: from molecular catalysts to surface oxides.*
- International Conference on Electronic Materials and Nanotechnology for Green Environment 2014 (ENGE2014), Jeju (South Korea), November 17-19 (2014), *DFT modeling of water oxidation: from molecular catalysts to surface oxides.*
- ICTP Workshop "Material Challenges in Devices for Solar Fuel Production and Employment", Trieste (Italy), May 19-23 (2014)*, DFT modeling of water oxidation: from molecular catalysts to surface oxides.*
- School on Numerical Methods for Materials Science Related to Renewable Energy Applications, ICTP, Trieste, Italy, November 26-30 (2012), *(i) First-principles modeling of electrochemical reactions for solar-to-fuel energy storage* and *(ii) Ab-initio modeling of Ru-based homogeneous catalysts for water oxidation.*

- Workshop on New Materials for Renewable Energy, ICTP, Trieste, Italy, September 17-21 (2011), *(i) First-principles modeling of electrochemical reactions for solar-to-fuel energy storage* and *(ii) Ab-initio modeling of Ru-based homogeneous catalysts for water oxidation.*
- Psi-k/CECAM workshop "Catalysis from First-Principles in Magleås, Denmark, May 22-26 (2011), *Ab-initio modelling of Ru-based homogeneous catalysts for water oxidation.*
- Psi-k/CECAM workshop "Catalysis from First-Principles" at the Erwin-Schrödinger-Institute (ESI) in Vienna, Austria, May 25-28 (2009), *The system chemistry of an alloy catalyst: insights from DFT calculations.*
- IWOM3 workshop at the Harnack House, Berlin, Germany, March 10-13 (2009), *The system chemistry of an alloy catalyst: insights from DFT calculations.*
- ICTP, Trieste, Italy, Roberto Car's 60th birthday symposium, June 21 (2007), *First-principles investigation of Ag-Cu alloy surfaces in an oxidizing environment*

Invited Seminars

- Fritz Haber Institute of the Max Planck Society, Berlin, Germany, 21 January 2020, *Theoretical modeling of α-Fe2O3 electrodes for photocatalytic water oxidation.*
- Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany, 21 November 2018, *Impurities and single-atom alloy elements in Ag catalysts: Insights from DFT simulations and in situ experiments.*
- Yonsei University, Department of Materials Science and Engineering, Seoul, South Korea, 21 November 2014, *The Ag catalyst for ethylene epoxidation: insights from DFT calculations.*
- University of Kathmandu, Department of Physics, Nepal, 10 October 2014, *DFT modeling of water oxidation: from molecular catalysts to surface oxides.*
- Fritz Haber Institute of the Max Planck Society, Berlin, Germany, 21 September 2012, *The structure of Ag-Cu and Co-Pi catalysts: insights from DFT calculations.*
- Politecnico di Milano, Department of Energy, Milan, Italy, 15 June 2012, *The system chemistry of an alloy catalyst: insights from DFT calculations.*
- Keio University, Department of Chemistry, Tokyo, Japan, 16 April 2008*, Density Functional Theory study of Ag-Cu alloy surfaces in an oxidizing environment.*
- King's College, Department of Physics, London, U.K., 16 January 2008, *First-principles investigation of Ag-Cu alloy surfaces in an oxidizing environment.*

List of Publications

1) Peer-Reviewed Papers

[58] H. N. Nong, L. J. Falling, A. Bergmann, M. Klingenhof, H. P. Tran, C. Spöri, R. Mom, J. Timoshenko, G. Zichittella, A. Knop-Gericke, **S. Piccinin**, J. Pérez-Ramírez, B. Roldan Cuenya, R. Schlögl, P. Strasser, D. Teschner, T. E. Jones
Key role of chemistry versus bias in electrocatalytic oxygen evolution
Nature 587, 408–413 (2020)
DOI: https://doi.org/10.1038/s41586-020-2908-2

[57] K. Schweinar, S. Beeg, C. Hartwig , C. Rajamathi, O. Kasian, M. Prieto, L. Tanase, D. Gottlob, **S. Piccinin**, D. Raabe, T. Schmidt, R. Schlögl, B. Gault, T. Jones, M. Greiner
Linking theory, in-situ and model experiments to determine the structure of 2D meta-stable oxides on bimetallic AgCu alloy catalysts
ACS Applied Materials & Interfaces, 12 (20), 23595–23605 (2020)
DOI: https://doi.org/10.1021/acsami.0c03963

[56] M. Ferri, J. Elliott, S. Fabris, **S. Piccinin**
Establishing best practices to model the electronic structure of CuFeO2 from first principles
Phys. Rev. B 101 (15), 155201 (2020)
DOI: https://doi.org/10.1103/PhysRevB.101.155201

[55] M. Lamoth, T. E. Jones, M. Plodinec, A. Machoke, M. Krämer, A. Karpov, F. Rosowski, **S. Piccinin**, R. Schlögl, E. Frei
*Nano catalysts unravel the selective state of Ag*Cat
ChemCat, 12(11) 2977-2988 (2020)
DOI: https://doi.org/10.1002/cctc.202000035

[54] M. Ferri, J. Elliott, M. Farnesi Camellone, S. Fabris, **S. Piccinin**
Thermodynamic stability and native point defects of CuFeO2 photocathodes in dry and electrochemical environments
J. Phys. Chem. C 123, 49, 29589–29598 (2019)
DOI: https://doi.org/10.1021/acs.jpcc.9b08957

[53] Y. Lykhach, **S. Piccinin,** T. Skála, M. Bertram, N. Tsud, O. Brummel, M. Farnesi Camellone, K. Beranová, A. Neitzel, S. Fabris, K. C. Prince, V. Matolín, Jörg Libuda
Quantitative analysis of the oxidation state of cobalt oxides by resonant photoemission spectroscopy
J. Phys. Chem. Lett. 10, 6129-6136 (2019)
DOI: https://doi.org/10.1021/acs.jpclett.9b02398

[52] **S. Piccinin**
The band structure and optical absorption of hematite (α-Fe2O3): a first-principles GW-BSE study
Phys. Chem. Chem. Phys. 21, 2957-2967 (2019)
DOI: https://doi.org/10.1039/C8CP07132B

[51] K. Ulman, E. Poli, N. Seriani, **S. Piccinin**, and R. Gebauer
Understanding the electrochemical double layer at the hematite/water interface: A first principles molecular dynamics study
J. Chem. Phys. 150, 041707 (2019)
DOI: https://doi.org/10.1063/1.5047930

[50] R. Wyrwich, T. E. Jones, S. Günther, W. Moritz, M. Ehrensperger, S. Böcklein, P. Zeller, A. Lünser, A. Locatelli, T. O. Menteş, M. Niño, A. Knop-Gericke, Robert Schlögl, **S. Piccinin**, J. Wintterlin
LEED-I(V) structure analysis of the (7 × √3)rect SO4 phase on Ag(111): Precursor to the active species of the Ag-catalyzed ethylene epoxidation
J. Phys. Chem. C 22(47) 26998–27004 (2018)
DOI: https://doi.org/10.1021/acs.jpcc.8b09309

[49] M. T. Greiner, T. E. Jones, S. Beeg, L. Zwiener, M. Scherzer, F. Girgsdies, **S. Piccinin**, M. Armbrüster, A. Knop-Gericke, R. Schlögl
Free-atom-like d-states in dilute bimetallic catalysts
Nature Chemistry 10, 1008–1015 (2018)
DOI: https://doi.org/10.1038/s41557-018-0125-5

[48] T. E. Jones, R. Wyrwich, S. Böcklein, E. Carbonio, M. Greiner, A. Klyushin, W. Moritz, A. Locatelli, T. Menteş, M. Niño, A. Knop-Gericke, R. Schlögl, S. Günther, J. Wintterlin, **S. Piccinin**
The selective species in ethylene epoxidation on silver
ACS Catalysis 8, 3844-3852 (2018)
DOI: https://doi.org/10.1021/acscatal.8b00660

[47] E. A. Carbonio, T. C.R. Rocha, A. Klyushin, I. Píš, E. Magnano, S. Nappini, **S. Piccinin**, A.Knop-Gericke, R. Schlögl, T. E. Jones

Are Multiple Oxygen Species Selective in Ethylene Epoxidation on Silver?
Chem. Sci. 9, 990-998 (2018)
DOI: https://doi.org/10.1039/C7SC04728B

[46] **S. Piccinin**, D. Rocca and M. Pastore
Role of solvent in the energy level alignment of dye-sensitized NiO interfaces
J. Phys. Chem. C 121, 22286-22294 (2017)
DOI: https://doi.org/10.1021/acs.jpcc.7b08463

[45] N. Ansari, K. Ulman, M. Farnesi Camellone, N. Seriani, R. Gebauer, and **S. Piccinin**
Hole localization in Fe2O3 from density functional theory and wavefunction-based methods
Phys. Rev. Materials 1, 035404 (2017)
DOI: https://doi.org/10.1103/PhysRevMaterials.1.035404

[44] V. Pfeifer, T.E. Jones, J. Velasco Vélez, R. Arrigo, **S. Piccinin**, M. Hävecker, A. Knop-Gericke and R. Schlögl
In situ observation of reactive oxygen species forming on oxygen-evolving iridium surfaces
Chem. Sci. 8, 2143-2149 (2017)
DOI: https://doi.org/10.1039/C6SC04622C

[43] **S. Piccinin** and M. Stamatakis
Steady-state CO oxidation on Pd(111): first-principles kinetic Monte Carlo simulations and microkinetic analysis
Topics in Catalysis 60, 141-151 (2017)
DOI: https://doi.org/10.1007/s11244-016-0725-5

[42] K. Ulman, M-T. Nguyen, N. Seriani, **S. Piccinin**, R. Gebauer
A unified picture of water oxidation on bare and gallium oxide covered hematite from density functional theory
ACS Catalysis 7, 1793-1804 (2017)
DOI: https://doi.org/10.1021/acscatal.6b03162

[41] T. Lee, Y. Lee, **S. Piccinin** and A. Soon
Ab initio thermodynamics of surface oxide structures undercontrolled growth conditions
J. Phys. Chem. C 121 (4), 2228–2233 (2017)
DOI: https://doi.org/10.1021/acs.jpcc.6b11445

[40] T. E. Jones, R. Wyrwich, S. Böcklein, T. C. R. Rocha, E. A. Carbonio, A. Knop-Gericke, R. Schlögl, S. Günther, J. Wintterlin, **S. Piccinin**
Oxidation of ethylene on oxygen reconstructed silver surfaces
J. Phys. Chem. C 120, 28630–28638 (2016)
DOI: https://doi.org/10.1021/acs.jpcc.6b10074

[39] V. Pfeifer, T. E. Jones, S. Wrabetz, C. Massué, J. Velasco-Velez, R. Arrigo, M. Scherzer, **S. Piccinin**, M. Hävecker, A. Knop-Gericke, R. Schlögl
Reactive oxygen species in iridium-based OER catalysts
Chem. Sci. 7, 6791-6795 (2016)
DOI: https://doi.org/10.1039/C6SC01860B

[38] C. Struzzi, C.S. Praveen, M. Scardamaglia, N.I. Verbitskiy, A.V. Fedorov, M. Weinl, M. Schreck, A. Grüneis, **S. Piccinin**, S. Fabris, and L. Petaccia
Controlled thermodynamics for tunable electron doping of graphene on Ir(111)
Phys Rev. B 94, 085427 (2016)
DOI: https://doi.org/10.1103/PhysRevB.94.085427

[37] V. Pfeifer, T.E. Jones, J.J. Velasco Vélez, C. Massué, R. Arrigo, D. Teschner, F. Girgsdies, M. Scherzer, M. Greiner, J. Allan, M. Hashagen, G. Weinberg, **S. Piccinin**, M. Hävecker, R. Schlögl, A. Knop-Gericke
The electronic structure of iridium and its oxides
Surface and Interface Analysis 48(5), 261-273, (2016)
DOI: https://doi.org/10.1002/sia.5895

[36] M. Stamatakis and **S. Piccinin**
Rationalising the relation between adlayer structure and observed kinetics in catalysis
ACS Catalysis 6, 2105–2111 (2016)
DOI: https://doi.org/10.1021/acscatal.5b02876

[35] V. Pfeifer, T. E. Jones, J. J. Velasco Vélez, C. Massué, R. Arrigo, D. Teschner, F. Girgsdies, M. Scherzer, J. Allan, M. Hashagen, G. Weinberg, **S. Piccinin**, M. Hävecker, R. Schlögl, A. Knop-Gericke
The Electronic Structure of Iridium Oxide Electrodes Active in Water Splitting
Phys. Chem. Chem. Phys. 18, 2292-2296 (2016)
DOI: https://doi.org/10.1039/C5CP06997A

[34] T. E. Jones, T. C. R. Rocha, A. Knop-Gericke, C. Stampfl, R. Schlögl and **S. Piccinin**
Insights into the electronic structure of the oxygen species active in alkene epoxidation on silver
ACS Catalysis 5, 5846-5850 (2015) (**ACS Editors' Choice**)
DOI: https://doi.org/10.1021/acscatal.5b01543

[33] A. Fedorov, C. S. Praveen, N. Verbitskiy, D. Haberer, D. Usachov, D. Vyalikh, A. Nefedov, C. Wöll, L. Petaccia, Luca; **S. Piccinin,** H. Sachdev, M. Knupfer, B. Buechner, S. Fabris, A. Grueneis
Efficient gating of epitaxial boron nitride monolayers by ionic functionalization
Phys. Rev. B 92, 125440 (2015)
DOI: https://doi.org/10.1103/PhysRevB.92.125440

[32] **S. Piccinin** and S. Fabris
Water Oxidation by Ru-Polyoxometalate Catalysts: Overpotential Dependency on the Number and Charge of the Metal Centers
Inorganics 3, 374-387 (2015)
DOI: https://doi.org/10.3390/inorganics3030374

[31] C.S. Praveen, **S. Piccinin** and S. Fabris
Adsorption of alkali adatoms on graphene supported by the Au/Ni(111) surface
Phys. Rev. B 92, 075403 (2015)
DOI: https://doi.org/10.1103/PhysRevB.92.075403

[30] C. Ma, L. Martin-Samos, S. Fabris, A. Laio, **S. Piccinin**
QMMMW: A wrapper for QM/MM simulations with Quantum ESPRESSO and LAMMPS
Comp. Phys. Comm. 195, 191-198 (2015)
DOI: https://doi.org/10.1016/j.cpc.2015.04.024

[29] A. Rossi, **S. Piccinin**, V. Pellegrini, S. de Gironcoli, V. Tozzini
Nano-scale corrugations in graphene: a Density Functional Theory based of structure, electronic properties and hydrogenation
J. Phys. Chem. C 119 (14), 7900-7910 (2015)
DOI: https://doi.org/10.1021/jp511409b

[28] T. E. Jones, T. C. R. Rocha, A. Knop-Gericke, C. Stampfl, R. Schlögl, and **S. Piccinin**
Thermodynamic and spectroscopic properties of oxygen on silver under an oxygen atmosphere
Phys. Chem. Chem. Phys. 17, 9288-9312 (2015)
DOI: https://doi.org/10.1039/C5CP00342C

[27] L. Dietz, **S. Piccinin** and M. Maestri
Mechanistic insights into the CO2 activation on metal surfaces
J. Phys. Chem. C 119, 4959-4966 (2015)
DOI: https://doi.org/10.1021/jp512962c

[26] M.-T. Nguyen, **S. Piccinin**, N. Seriani and R. Gebauer
Photo-oxidation of water on defective hematite(0001)
ACS Catalysis 5, 715-721 (2015)
DOI: https://doi.org/10.1021/cs5017326

[25] **S. Piccinin** and M. Stamatakis
CO oxidation on Pd(111): a first-principles based kinetic Monte Carlo study
ACS Catalysis 4, 2143-2152 (2014)
DOI: https://doi.org/10.1021/cs500377j

[24] C. Ma, **S. Piccinin** and S. Fabris
Rigid- and polarizable-ion potentials for modeling Ru-polyoxometalate catalysts for water oxidation
Acta Chim. Slo. 61, 302-307 (2014)

[23] T. E. Jones, T. C. R. Rocha, A. Knop-Gericke, C. Stampfl, R. Schlögl, and **S. Piccinin**
Adsorbate induced vacancy formation on silver surfaces
Phys. Chem. Chem. Phys. 16, 9002-9014 (2014)
DOI: https://doi.org/10.1039/C4CP00778F

[22] M. Fronzi, **S. Piccinin**, B. Delley, E. Traversa and C. Stampfl
CHx adsorption (x=1-4) and thermodynamic stability on the CeO2 (111) surface: A first-principles investigation
RSC Advances 4, 12245-12251(2014)
DOI: https://doi.org/10.1039/C4RA01224K

[21] M.-T. Nguyen, N. Seriani, **S. Piccinin** and R. Gebauer
Photo-driven oxidation of water on alpha-Fe2O3 surfaces: an ab-initio study
J. Chem. Phys. 140, 064703 (2014)

DOI: https://doi.org/10.1063/1.4865103

[20] C. Ma, **S. Piccinin** and S. Fabris
Interface structure and reactivity of water-oxidation Ru–polyoxometalate catalysts on functionalized graphene electrodes
Phys. Chem. Chem. Phys. 16, 5333-5341 (2014)
DOI: https://doi.org/10.1039/C3CP54943G

[19] K. Kwapien, **S. Piccinin** and S. Fabris
Energetics of Water Oxidation Catalyzed by Cobalt Oxide Nanoparticles: Assessing the Accuracy of DFT and DFT+U Approaches Against Coupled Cluster Methods
J. Phys. Chem. Letters 4, 4223–4230 (2013)
DOI: https://doi.org/10.1021/jz402263d

[18] D. Haberer, L. Petaccia, A. V. Fedorov, C. S. Praveen, S. Fabris, **S. Piccinin**, O. Vilkov, D. V. Vyalikh,A. Preobrajenski, N. I. Verbitskiy, H. Shiozawa, J. Fink, M. Knupfer, B. Buchner and A. Grueneis
Anisotropic Eliashberg function and electron-phonon coupling in doped graphene
Phys. Rev. B 88, 081401(R) (2013)
DOI: https://doi.org/10.1103/PhysRevB.88.081401

[17] T.E. Jones, **S. Piccinin** and C. Stampfl
Relativity and nobility of gold
Mat. Chem. Phys. 141, 14-17 (2013)
DOI: https://doi.org/10.1016/j.matchemphys.2013.04.049

[16] L.N. Nguyen, S. de Gironcoli and **S. Piccinin**
Ag-Cu catalysts for ethylene epoxidation: Selectivity and activity descriptors
J. Chem. Phys. 138, 184707 (2013)
DOI: https://doi.org/10.1063/1.4803157

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