Curriculum Vitae

A Personal Data

Surname	Franchini
Name	Cesare
Place of Birth	Modena, Italy
Date of Birth	October 3rd, 1975
Citizenship	Italian
Marital status	Married, one child
Contact Vienna	Faculty of Physics, University of Vienna Computational Materials Physics Kolingasse 14-16/03.65, A-1090 Vienna, Austria phone: +43 1 4277 73315 email: cesare.franchini@univie.ac.at web: `http://homepage.univie.ac.at/cesare.franchini/`
Contact Bologna	Dipartimento di Fisica e Astronomia "Augusto Righi" Alma Mater Studiorum - Universita di Bologna Viale Berti Pichat 6/2, 40127 Bologna, Italy phone: +39 051 20 9 5145 email: cesare.franchini2@unibo.it web: `https://www.unibo.it/sitoweb/cesare.franchini2/`
Research ID	B-2084-2009
ORCID	0000-0002-7990-2984

B Education

2002, PhD Physics	Technical University of Vienna (Austria) *excellent*
1999, MS Physics	University of Cagliari (Italy) 110/110 *cum laude*

C Career History

From 2017	Full Professor, *Quantum Materials Modelling*, University of Vienna (Austria)
From 2018	Associate Professor, University of Bologna (Italy)
2014 - 2017	Associate Professor, University of Vienna (Austria)
2012 - 2014	Assistant Professor (Tenure Track), University of Vienna (Austria)
2013	Parental Leave
2007 - 2012	University Assistant, University of Vienna (Austria)
2004 - 2007	PostDoc, University of Vienna (Austria)
2002 - 2004	PostDoc, University of Cagliari (Italy)

C.1 Esteem Factors

2017	Shield of honor, Abbottabad University, Pakistan
2017	National Scientific Habilitation (Italy), Full Prof. Sector: 02/B2 - Theoretical physics of matter
2015	Outstanding Referee, American Physical Society
2013	National Scientific Habilitation (Italy), Assoc. Prof. Sector: 02/B2 - Theoretical physics of matter
2010	Young International Scientist Fellowship, Chinese Academy of Sciences

Referee	Deutsche Forschungsgemeinschaft (DFG) Department of Energy, DOE (USA) The Velux Foundations (Denmark) USA-Israel Binational Science Foundation (USA) Czech Science Foundation (GACR, Czech Republic) FONDECYT (Chile)

D Main Scientific Interests

My research is concerned with the theoretical understanding and computational modeling of complex materials using quantum mechanical methodologies based on Density Functional Theory (DFT), Hartee-Fock, Many-body perturbation theory (GW, RPA, BSE), Diagrammatic Monte Carlo, model effective Hamiltonians, molecular dynamics and machine learning. Computational quantum materials: spin-orbit coupled correlated materials, non-collinear magnetism, insulator-to-metal transitions; Computational surface science: energetics, catalysis, defects, polarity; Polaron physics: formation, dynamics, quasi-particle many-body properties.

E Publications

E.1 Bibliometric Data (updated 18/06/2020)

143 papers	ISI	Google Scholar
h-index	36	41
Citations	4788	7563

E.2 Selected Publications [10]

The full list of publications is given in [K].

1. *Polarons in Materials*, C. Franchini, M. Reticcioli, M. Setvin, U. Diebold,
   Nat. Rev. Mater. (2021). DOI: `https://doi.org/10.1038/s41578-021-00289-w`

2. *Unravelling CO Adsorption on Model Single-Atom Catalysts* J. Hulva, M. Meier, R. Bliem, Z. Jakub, F. Kraushofer, M. Schmid, U. Diebold, C. Franchini, G. S. Parkinson,

   Science 371, 375 (2021). DOI: https://doi.org/110.1126/science.abe5757

3. *Polarity compensation mechanisms on the perovskite surface $KTaO_3$ (001)* M. Setvin, M. Retticioli, F. Polzleitner, J. Hulva, M. Schmid, C. Franchini, U. Diebold,

   Science 359, 572 (2018). DOI: https://doi.org/10.1126/science.aar2287

4. *Tunable metal-insulator transition, Rashba effect and Weyl Fermions in a relativistic charge-ordered ferroelectric oxide* J. He, D. Di Sante, R. Li, X. Chen, J.M. Rondinelli, C. Franchini,

   Nature Communications 9, 492 (2018). DOI: https://doi.org/10.1038/s41467-017-02814-4

5. *Anisotropy of magnetic interactions and symmetry of the order parameter in unconventional superconductor Sr2RuO4* B. Kim, S. Khmelevskyi, I. Mazin, D. Agterberg, C. Franchini,

   npj Quantum Materials, 3 37 (2017). DOI: https://doi.org/10.1038/s41535-017-0041-8

6. *Polaron-Driven Surface Reconstructions* M. Reticcioli, M. Setvin, X. Hao, P. Flauger, G. Kresse, M. Schmid, U. Diebold, C. Franchini,

   PRX 7, 031053 (2017) DOI: https://doi.org/10.1103/PhysRevX.7.031053

7. *Anisotropic magnetic couplings and structure-driven canted to collinear transitions in Sr_2IrO_4 by magnetically constrained noncollinear DFT*, P. Liu, S. Khmelevskyi, B. Kim, M. Marsman, D. Li, XQ Chen, D.D. Sarma, G. Kresse, C. Franchini,

   Phys. Rev. B **91**, 085204 (2015). DOI: http://dx.doi.org/10.1103/PhysRevB.92.054428

8. *Direct View at Excess Electrons in TiO_2 Rutile and Anatase* M. Setvin, C. Franchini, X. Hao, M. Schmid, A. Janotti, M. Kaltak, C. G. Van de Walle, G. Kresse, U. Diebold

   Phys. Rev. Lett. 113, 086402 (2014). DOI: https://doi.org/10.1103/PhysRevLett.113.086402

9. *Dirac semimetal and topological phases in A_3Bi (A=Na, K, Rb)*, Z. Wang, Y. Sun, X.-Q. Chen, C. Franchini, G. Xu, H. Weng, X.Dai, and Z. Fang,

   Phys. Rev. B **85**, 195320 (2012). DOI: 10.1103/PhysRevB.85.195320

10. *Polaronic hole-trapping in doped $BaBiO_3$* C. Franchini, G. Kresse and R. Podloucky

    Phys. Rev. Lett. 102, 256402 (2009). DOI: https://doi.org/10.1103/PhysRevLett.102.256402

F Selected Talks

About 60 ($\sim$ 30 invited/key-note) talks & seminars. See full list of invited talks [L].

1. *Polarons in the gap*
   EMRS fall meeting;
   Warsaw (Poland), September 20-23 2021.

2. *Predicting properties of complex materials: electrons and quasielectrons*
   EMRS fall meeting;
   Warsaw (Poland), September 17-20 2018.

3. *Hybrid functionals for simulating complex oxides*
   APS March Meeting;
   Baltimore (USA), March 2016.

4. *Electronic Structure of Perovskites: Lessons from Hybrid Functionals*
   Autumn School on Correlated Electrons
   Forschungszentrum Jülich (Germany), Sept. 2015.

5. *Small and Large Polarons in TiO2 Rutile and Anatase surfaces*
   MRS Fall Meeting;
   Boston (USA), December 2014.

6. *Screened hybrid density functionals applied to 3d, 4d, and 5d transition metal perovskites*
   Joint European Magnetic Symposia;
   Parma (Italy), June 2012.

7. *Multivalency and polaronic hole trapping in $BaBiO_3$*
   APS March Meeting;
   Portland (USA), March 2010.

G Teaching

The focus of my teaching activity is *Computational Physics* and *Materials Physics* at all levels of studies (Bachelor, Master and PhD).

- Electronic structure of Materials: Master in Physics (University of Vienna)
- Computational Physics: Master "Computational Science" (University of Vienna)
- Practicum in Computational Quantum Mechanics: Bachelor in Physics (University of Vienna)
- Practicum in Computational Materials Physics: Master in Physics (University of Vienna)
- Seminars on quantum Materil Modelling: Master in Physics (University of Vienna)

- Physics of Matter: Bachelor in Physics (University of Bologna)
- Computational Materials Physics: Master in Physics (University of Bologna)
- Interactions & Correlations: Master in Physics (University of Bologna)

H Supervision

> 50 PostDoc, PhD, MS and Bachelor students supervised.
The full list of publications is given in [L].

I Self-active acquired third-party found projects

1. **COST action**

   Title: "Advancing knowledge on physics, materials and chemical processes".

   Duration: 3 years (End 2021-2024).

   Role: Management Committee member.

   Funding Agency: EU-funded.

   Budget: travel and networking.

2. **FWF Spezialforschunbereich Project.**

   Title: "Taming Complexity in Materials Modeling".

   Duration: 4 years (2021- 2015).

   Role: sub-Project P.I.

   Funding Agency: Austrian Science Founds (FWF, Austria).

   Budget: 400.00,00 EURO.

3. **OeAD WTZ Austria-Korean exchange program.**

   Title: "Novel properties of correlated oxide surfaces"

   Duration: 2 years (2020-2022).

   Role: P.I.

   Funding Agency: OeaD, Austria).

   Budget: 15.000,00 EURO

4. **FWO-FWF Austrian-Belgium International Research Project.**

   Title: "Ab-initio calculations for anharmonic polarons in hydrides"

   Duration: 4 years (2020-2024).

   Role: P.I.

   Funding Agency: Austrian Science Founds (FWF, Austria).

   Budget: 400.000,00 EURO

5. **H2020-MSCA-IF-2019.**

   Title: "aB-IniTio calculations and MAchine learning for suPerconducting collective phenomena in novel materials"

   Duration: 3 years (2020-2024).

   Role: supervisor (winner: Dr. Domenico di Sante)

   Funding Agency: H2020

   Budget: 269.000,00 EURO

6. **doc.funds "Hierarchical Design of Hybrid Systems"**

   Title of subproject: Spin-orbit effects in defective van der Waals heterostructures

   Role: Subproject P.I.

   Funding Agency: Austrian Science Founds (FWF, Austria).

   Budget required: 1 PhD student for 3.5 years (2021-2024)

7. **FWF Research Project.**

   Title: "Surface science of bulk-terminated cubic perovskite oxides (SUPER)"

   Duration: 3.5 years (2019-2023).

   Role: co-P.I.

   Funding Agency: Austrian Science Founds (FWF, Austria).

   Budget: 130.000,00 EURO

8. **Exchange I-LINK2017 program, CSIC (Spain-Austria)**

   Title: " Interplay between relativistic and electronic correlation effects in complex oxides "

   Duration: 2 years (2018-2020).

   Role: Austrian P.I.

   Funding Agency: CSIC (Spain).

   Budget: 20.000,00 EURO.

9. **Belgium-Austria Joint Research Project.**

   Title: "Polarons in oxides: model Hamiltonian and ab initio study"

   Duration: 3 years (2016-2019).

   Role: Austrian P.I.

   Funding Agency: Austrian Science Founds (FWF, Austria).

   Budget: 330.000,00 EURO.

10. **FWF Spezialforschunbereich Project.**

    Title: "Collective Phenomena in Oxide films and Heterostructures".

    Duration: 3.5 years (2015- 2018).

    Role: Project Partner.

    Funding Agency: Austrian Science Founds (FWF, Austria).

    Budget: 125.650,00 EURO.

11. **COST action**

    Title: "Towards Oxide Based Electronics".

    Duration: 3 years (End 2014-2017).

    Role: Management Committee member.

Funding Agency: EU-funded.

Budget: travel and networking.

12. **India-Austria Joint Research Project.**

    Title: "Electron correlation and spin-orbit coupling in $4d$ and $5d$ transition metal oxides: a joint experimental and theoretical frontier research".

    Duration: 3 years (2014-2017).

    Role: Austrian P.I.

    Funding Agency: Austrian Science Founds (FWF, Austria).

    Budget: 350.000,00 EURO.

13. **Collaboration within the FWF START Grant (P.I:: Gareth Parkinson).**

    Title: "Unravelling Single-Atom Catalysis: A Surface-Science Approach".

    Duration: 2 years (2016-2018).

    Role: Project Collaborator (external)

    Funding Agency: FWF.

    Budget: 120.000,00 EURO (1 Post-Doc position)

14. **Collaboration within the ERC Advanced Research Grant (P.I:: Ulrike Diebold).**

    Title: "OxideSurfaces".

    Duration: 2 years (2012-2014).

    Role: Project Collaborator (external)

    Funding Agency: European Research Council.

    Budget: 120.000,00 EURO (1 Post-Doc position)

15. **FP7 Collaborative Projects (EU-India-2)**

    Title: "Advanced Theories for functional oxides: new routes to handle the devices of the future";

    Duration: 3 years (2009-2012).

    Role: Austrian P.I.

    Funding Agency: EU-funded.

    Budget: 250.000,00 EURO

16. **International (Regional) Cooperation and Exchange Program**

    Title: Modeling complex strongly correlated oxides;

    Duration: 1 year (2010).

    Role: P. I.

    Funding Agency: National Science Fundation China.

    Budget: 22.870,00 EURO.

J Organizational Activity

2021 South Korea - Austria mini Symposium
Workshop, Vienna, September 2021

2019 Novel Electronic and Magnetic Phases in Correlated Spin
Workshop, Mainz, November 2019

2019 Polaron in the 21^{st} century
Workshop, Vienna, December 2019

2019 South Korea - Austria mini Symposium
Workshop, Vienna, November 2019

2019 Computational Approaches to Magnetic Systems
Workshop, Daejeon (South Korea, August 2019

2018 Computational Magnetism
Workshop, POSTECH, August 2018

2017 Computational Magnetism
Workshop, POSTECH, August 2018

2017 International Conference on Strongly Correlated Electron Systems
Symposium: "Novel electronic and magnetic phases in correlated relativistic oxides"
Prague (Czech Republic)

2017 Winter School of Magnetism
Vienna (Austria)

2016 17th International conference of the Asia Materials Sciences
Qingdao (China)

2015 1st International Conference on Computational Designs and Simulations of Materials
Shenyang (China)

2014 Symposium: *Computational Materials Methods. Design and Applications*
International Conference of Young Researchers on Advances Materials;
Haikou (China)

2012 School: *ATHENA School for advanced modeling of magnetic oxides*
Calcutta (India)

K Editorial Activity

2021 Festschrift for Prof. Sandro Massidda: Novel superconducting and magnetic materials
J. of Phys.: Condens. Mat. (2020)
Co-editor

2020 Handbook of Materials Modeling
Springer
Co-editor

2019 Novel Superconducting and Magnetic Materials,
J. Physics: Condens. Matter
Co-editor

L List of supervised students and postDOC

Type	Name	Topic	Period
Post-Doc	Michele Reticcioli	Polarons	2019-
Post-Doc	Liang Si	Strongly correlatied oxides	2017-2018
Post-Doc	Matthias Meier	Computational Surface Science	2016-
Post-Doc	Bongjae Kim	Relativistic Oxides	2014-2017
Post-Doc	Xianfeng Hao	Computational Surface Science	2012-2015
Post-Doc	Jiangang He	Hybrid functional for oxides	2011-2013
PhD	Viktor Birschitzky	*Machine Learning for Polarons*	2020-
PhD	Florian Ellinger	*Quantum paraelectric surfaces*	2020-
PhD	Panukorn Sombut	*Single atom catalysis*	2020-
PhD	Lorenzo Varrassi	*High throughput BSE*	2019-
PhD	Dario Fiore Mosca	*Multipolar Magnetism*	2019-
PhD	Thomas Hahn	*Diagrammatic MC*	2017-
PhD	Michele Reticcioli	*Polarons in rutile TiO_2*	2015-
PhD	Zeynep Ergonenc	*GW for Perovskites*	2014-2018
PhD	Peitao Liu	*Spin-orbit coupling in Iridates*	2013-2017
PhD	Sowmya S. Murthy	*$RMnO_3$: ab initio + Hamiltonian*	2010-2013
PhD (co-supervisor)	Veronika Bayer	*MnO surfaces*	2004-2007
PhD (visiting)	Muhmmad Shafiq	*Polarons in $SrTiO_3$(100) surface*	03-07 2015
PhD (visiting)	Sun Yan	*Topological Insulators*	2012
Master	Josef Huber	*Phonons of quantum paraelectric perovskites*	2021-
Master	David Dirnberger	*Band Unfolding scheme in VASP*	2021-
Master	Marco Corrias	*Polaorn MD*	2021-
Master	Lorenzo Celiberti	*Spin-orbit coupled Polaorns*	2021-
Master	Stefano Ragni	*Diagrammatic Monte Carlo*	2020
Master	Luigi Rannali	*Anharmonic phonons*	2021
Master	Andrea Angeletti	*Polaron in WO_3*	2021
Master	Viktor Birschitzky	*Machine Learning for polarons*	2020
Master	Florian Ellinger	*GW database*	2020
Master	Lorenzo Varrassi	*BSE for perovskites*	2018
Master	Dario Fiore Mosca	*Quantum Magnetism*	2018
Master	Sabine Dobrowitz	*Electron doping in $NaOsO_3$*	2017
Master	Thomas Hahn	*Diagrammatic Monte Carlo*	2016-2017
Master (co-supervisor)	Antonio Sanna	*Strongly correlated oxides*	2003-2004

M Publication List

141. *Optical and excitonic properties of transition metal oxide perovskites by the Bethe-Salpeter equation* Lorenzo Varrassi, Peitao Liu, Ergonenc Yavas, Menno Bokdam, Georg Kresse, and Cesare Franchini, Phys. Rev. Mat., accepted (2021)

140. *Pressure-induced excitations in the out-of-plane optical response of the nodal-line semimetal ZrSiS* J. Ebad-Allah, S. Rojewski, M. Vst, G. Eickerling, W. Scherer, E. Uykur, R. Sankar, L. Varrassi, C. Franchini, K. Ahn, J. Kunes, C. A. Kuntscher, Physical Review Letter, accepted (2021)

139. *Electronic state unfolding for plane waves: energy bands, Fermi surfaces and spectral functions* David Dirnberger, Georg Kresse, Cesare Franchini, and Michele Reticcioli, J. Phys. Chem. C 125, 23, 12921-12928 (2021) DOI: 10.1021/acs.jpcc.1c02318

138. *Nanoscale synthesis of ionic analogues of bilayer silicene with high carrier mobility* D. Averyanov, P. Liu, I. Sokolov, O. Parfenov, I. Karateev, D. Di Sante, C. Franchini, A. Tokmachev, V. Storchak, J. Mater. Chem. C 2021 DOI: 10.1039/D1TC01951A

137. *Polarons in Materials* Cesare Franchini, Michele Reticcioli, Martin Setvin, Ulrike Diebold, Nature Review Materials (2021) DOI:10.1038/s41578-021-00289-w

136. *Advanced First-Principles Modeling of Relativistic Ruddlesden-Popper Strontium iridates* P. Liu and C. Franchini, Appl. Sci. 2021, 11(6), 2527 DOI: 10.3390/app11062527

135. *Interplay between multipolar spin interactions, Jahn-Teller effect and electronic correlation in a Jeff=3/2 insulator* Dario Fiore Mosca, Leonid V. Pourovskii, Beom Hyun Kim, Peitao Liu, Samuele Sanna, Federico Boscherini, Segii Khmelevskyi, Cesare Franchini, Physical Review B 103, 104401 (2021) DOI: 10.1103/PhysRevB.103.104401

134. *Magnetic 3d adatoms on free-standing and Ni(111)-supported graphene* Florian Ellinger, Cesare Franchini, Valerio Bellini, Phys. Rev. M 5, 014406 (2021) DOI: 10.1103/PhysRevMaterials.5.014406

133. *Unravelling CO Adsorption on Model Single-Atom Catalysts* Jan Hulva, Matthias Meier, Roland Bliem, Zdenek Jakub, Florian Kraushofer, Michael Schmid, Ulrike Diebold, Cesare Franchini, Gareth S. Parkinson, Science 371, 375 (2021), DOI:10.1126/science.abe5757

132. *Osmates on the verge of a Hunds-Mott transition: The different fates of NaOsO3 and LiOsO3* Daniel Springer, Bongjae Kim, Peitao Liu, Sergii Khmelevskyi, Massimo Capone, Giorgio Sangiovanni, Cesare Franchini, and Alessandro Toschi, Phys. Rev. Lett. 125, 166402 (2020) DOI: 10.1103/PhysRevLett.125.166402

131. *Aberrant electronic and structural alterations in pressure tuned perovskite NaOsO3* Raimundas Sereika, Peitao Liu, Bongjae Kim, Sooran Kim, Jianbo Zhang, Bijuan Chen, Kazunari Yamaura, Changyong Park, Cesare Franchini, Yang Ding, Ho-kwang Mao npj Quantum Materials volume 5, 66 (2020) DOI:10.1038/s41535-020-00269-3

130. *Doping evolution of the local electronic and structural properties of the double perovskite Ba2Na(1-x)Ca(x)OsO6* Jagadesh Kopula Kesavan, Dario Fiore Mosca, Samuele Sanna, Francesco Borgatti, Gtz Schuck, Phoung M. Tran, Patrick M. Woodward, Vesna F. Mitrovic, Cesare Franchini, and Federico Boscherini, J. Phys. Chem. C 124, 30, 16577-16585 (2020) DOI: 10.1021/acs.jpcc.0c04807

129. *CuAu, a hexagonal two-dimensional metal* Georg Zagler, Michele Reticcioli, Clemens Mangler, Daniel Scheinecker, Cesare Franchini, and Jani Kotakoski, 2D Mater. 7 045017 (2020) DOI: 10.1088/2053-1583/ab9c39

128. *Mimicking superconductivity of Sr2RuO4 through superlattice engineering* Bongjae Kim, Sergii Khmelevskyi, Cesare Franchini, Igor Mazin, Kyoo Kim, Phys. Rev. B 101, 220503(R) (2020) DOI: 10.1103/PhysRevB.101.22050

127. *Resolving the adsorption of molecular O2 on the rutile TiO2(110) surface by non-contact atomic force microscopy* Igor Sokolovic, Michele Reticcioli, Martin Calkovsky, Margareta Wagner, Michael Schmid, Cesare Franchini, Ulrike Diebold, Martin Setvin, PNAS 117 (26) 14827-14837 (2020) DOI:10.1073/pnas.1922452117

126. *Electron-Phonon Interactions Using the PAW Method and Wannier Functions* Manuel Engel, Martijn Marsman, Cesare Franchini, Georg Kresse, Phys. Rev. B 101, 184302 (2020) DOI:10.1103/PhysRevB.101.184302

125. *Tunable Relativistic Quasiparticle Electronic and Excitonic Behavior of the FAPb(I1-xBrx)3 Alloy* Zeeshan Muhammd, Peitao Liu, Rashid Ahmad, Saeid Jalali Asadabadi, Cesare Franchini, Iftikhar Ahmad, PCCP 22, 11943-11955 (2020) DOI: 10.1039/D0CP00496K

124. *Comparative ab initio study of the structural, electronic, magnetic, and dynamical properties of LiOsO3 and NaOsO3* Peitao Liu, Jiangang He, Bongjae Kim, Sergii Khmelevskyi, Alessandro Toschi, Georg Kresse, Cesare Franchini, Phys. Rev. Materials 4, 045001 (2020) DOI: 10.1103/PhysRevMaterials.4.045001

123. *Optical response of an interacting polaron gas in strongly polar crystal* Serghei Klimin, Jacques Tempere, Jozef Devreese, Cesare Franchini, Georg Kresse, Appl. Sci. 10(6), 2059 (2020) DOI: 10.3390/app10062059

122. *Kagome Metal-Organic Frameworks as a Platform for Strongly Correlated Electrons* Domenico Di Sante, Marius Fuchs, Peitao Liu, Tilman Schwemmer, Giorgio Sangiovanni, Ronny Thomale, Cesare Franchini, DOI: 10.1088/2515-7639/ab713b

121. *Probing structural changes upon carbon monoxide coordination to single metal adatom* P. T. P. Ryana, M. Meier, Z. Jakubc, J. Balajka, J. Hulva, D.J. Payne, T. L. Lee, C.Franchini, F. Allegretti, G. S. Parkinson, D. A. Duncan, J. Chem. Phys. 152, 051102 (2020) DOI: 10.1063/1.5137904

120. *Predicting the band gap of complex materials: computational methods and procedures.* F. Belviso *et al.*, Inorg. Chem. 58, 22, 14939-14980 (2019) DOI: 10.1021/acs.inorgchem.9b01785

119. *Preface: Special Issue on novel superconducting and magnetic materials* Memorial issues for Prof. Sandro Massidda F. Bernardini, L. Boeri, A. Floris, C. Franchini, G. Profeta, A. Sanna J. of Phys.: Condens. Mat. (2019) DOI: 10.1088%2F1361-648x%2Fab4cbe

118. *Cubic and tetragonal perovskites from the random phase approximation* Fanhao Jia, Georg Kresse, Cesare Franchini, Peitao Liu, Jian Wang, Alessandro Stroppa, and Wei Ren Phys. Rev. Materials 3, 103801 (2019) DOI: 10.1103/PhysRevMaterials.3.103801

117. *Assessing model-dielectric-dependent hybrid functionals on the antiferromagnetic transition-metal monoxides MnO, FeO, CoO, and NiO* Peitao Liu, Cesare Franchini, Martijn Marsman, and Georg Kresse J. Phys.: Condens. Matter 32 015502 (2020) DOI: 10.1088/1361-648X/ab4150

116. *Parameterisation of an LSDA+U model for non-collinear magnetic configurations: Multipolar magnetism in UO2* S. L. Dudarev, P. Liu, D. A. Andersson, C. R. Stanek, T. Ozaki, C. Franchini Phys. Rev. Materials 3, 083802 (2019) DOI: https:/doi.org/10.1103/PhysRevMaterials.3.083802

115. *Local Structure and Coordination Effects Define Adsorption in a Model Ir1/Fe3O4 Single-Atom Catalyst* Zdenek Jakub, Jan Hulva, Matthias Meier, Roland Bliem, Florian Kraushofer, Martin Setvin, Michael Schmid, Ulrike Diebold, Cesare Franchini, Gareth S. Parkinson Angew.Chem.Int.Ed. 58, 13961-13968 (2019) DOI: 10.1002/anie.201907536

114. *The Influence of Local Defects on the Dynamics of O-H Bond Breaking and Formation on a Magnetite Surface* Alexander Bourgund, Barbara A. J. Lechner, Matthias Meier, Cesare Franchini, Gareth, S. Parkinson, Ueli Heiz and Friedrich Esch J. Phys. Chem. C 123, 32, 19742-19747 (2019) DOI: https:/doi.org/10.1021/acs.jpcc.9b05547

113. *Intriguing Electronic and Optical Properties of M2CX2 (M=Mo,W; X=O, F) MXenes and their van der Waals heterostructures* S. A. Khan, Gul Rehman,, Iftikhar Ahmad, Cesare Franchini, B. Amin. Chemical Physics Letters 731, 136614 (2019) DOI: https:/doi.org/10.1016/j.cplett.2019.136614

112. *Defect chemistry of Eu dopants in NaI scintillators studied by atomically resolved force microscopy* Manuel Ulreich, Lynn A. Boatner, Igor Sokolovic, Michele Reticcioli, Flora Poelzleitner, Cesare Franchini, Michael Schmid, Ulrike Diebold, and Martin Setvin Phys. Rev. Materials 3, 075004 (2019) DOI: https://doi.org/10.1103/PhysRevMaterials.3.075004

111. *Spin fluctuation induced Weyl semimetal state in the paramagnetic phase of EuCd2As2* J.-Z. Ma, S. M. Nie, C. J. Yi, J. Jandke, T. Shang, M. Y. Yao, M. Naamneh, L. Q. Yan, Y. Sun, A. Chikina, V. N. Strocov, M. Medarde, M. Song, Y.-M. Xiong, G. Xu, M. Reticcioli, C. Franchini, C. Mudry, M. Mller, W. Wulfhekel, J. Mesot, Y. G. Shi, T. Qian, H. Ding, M. Shi Science Advances, 5 eaaw4718 (2019) DOI: https:/doi.org/10.1126/sciadv.aaw4718

110. *Doping-induced insulator-metal transition in the Lifshitz magnetic insulator NaOsO3* Sabine Dobrovits, Bongjae Kim, Michele Reticcioli, Alessandro Toschi, Sergii Khmelevskyi, and Cesare Franchini, J. Phys.: Condens. Matter31 244002 (2019) DOI:https://doi.org/10.1088/1361-648X/ab0dc4

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10. *Density functional theory study of MnO by an hybrid functional approach*, C. Franchini, V. Bayer, R. Podloucky, J. Paier, and G. Kresse, Phys. Rev. B **72**, 045132 (2005).

9. *Superconducting properties of MgB_2 from first principles*, A. Floris, G. Profeta, N. Lathiotakis, M. Lueders, M. Marques, C. Franchini, E.K.U. Gross, A. Continenza, and S. Massidda, Phys. Rev. Lett. **94**, 037004 (2005). [Selected for Virtual Journal of Applications of Superconductivity, **8**(3)]

8. *Role of electronic correlations on the ground state properties and on the pressure-induced metal-insulator transition in $BaVS_3$*, A. Sanna, C. Franchini, S. Massidda, and A. Gauzzi, Phys. Rev. B **70**, 235102 (2004).

7. *First stage Mn adsorption on clean Ge(111) surface*, G. Profeta, S. Picozzi, A. Continenza, and C. Franchini, Phys. Rev. B **70**, 155307 (2004).

6. *(3×1)-Br/Pt(110) structure and the charge-density-wave-assisted c(2×2) to (3×1) phase transition*, C. Deisl, K. Swamy, N. Memmel, E. Bertel, C. Franchini, G. Schneider, J. Redinger, S. Walter, L. Hammer, and K. Heinz, Phys. Rev. B **69**, 195405 (2004).

5. *Electronic structure of $PbFe_{\frac{1}{2}}Ta_{\frac{1}{2}}O_3$: crystallographic ordering and magnetic properties*, N. Lampis, C. Franchini, G. Satta, A. Geddo-Lehmann, and S. Massidda, Phys. Rev. B **69**, 064412 (2004).

4. *Chemical pressure induced ferromagnetism and stabilization of the metallic state in $Ba_{1-x}VSr_xS_3$*, A. Gauzzi, F. Licci, N. Barišić, G.L. Calestani, F. Bolzoni, E. Gilioli, M. Marezio, A. Sanna, C. Franchini, and L. Forró, W. Sc. Int. J. of Mod. Phys. B **17**, 3503. (2003). [Conference paper]

3. *Coverage dependent bromine adsorption on the Pt(110) surface*, C. Franchini, J. Redinger, C. Deisl, K. Swamy, E. Bertel, V. Blum, L. Hammer, and K. Heinz, 7^{th} International Conference on Nanometer-Scale Science and Technology and 21^{st} European Conference on Surface Science. Lund Univ. 2002, Sweden. [Conference paper]

2. *Structural, transport and electronic properties of $AuVS_2$, a new layered dichalcogenide with semimetallic properties*, A. Gauzzi, E. Gilioli, F. Licci, M. Marezio, G. Calestani, C. Franchini, and S. Massidda, Phys. Rev. B **66**, 085106 (2002).

1. *Structure of the c(2×2)-Br/Pt(110) surface*, V. Blum, L. Hammer, K. Heinz, C. Franchini, J. Redinger, K. Swamy, C. Deisl, and E. Bertel, Phys. Rev. B **65**, 165408 (2002).

0. *Structural and Electronic Properties of $HgBa_{2-x}Sr_xCuO_{4+\delta}$*, C. Franchini, S. Massidda, A. Continenza, and A. Gauzzi, Phys. Rev. B **62**, 9163 (2000).

N Invited Talks

32. Quantum Surfaces ZCAM-ASEVA Workshop on Metal-oxide ultrathin films and nanostructures;
Zaragoza, Spain, July 6-10 2020 → postponed to July 5-9, 2022

31. Polarons in the gap 2020 E-MRS Fall Meeting, Warsaw;
September 2020 ⇒ moved to 2021

30. Diagrams and tensors in Computational (Materials) Physics
Seminars on particle physics;
University of Vienna
May 29 2020.

29. *Quantum Materials by DFT*
Korea Institute for Advanced Study (KIAS);
Seoul (South Korea), August 30 2019.

28. *Electron-lattice interactions in (quantum) oxide surfaces*
University of Hamburg - SFB986;
Hamburg (Germany), June 21 2019.

27. *Computational Quantum Materials: Protocols & Examples*
University of Duisburg;
Duisburg (Germany), June 18 2019.

26. *Predicting properties of complex materials: electrons and quasielectrons*
EMRS fall meeting;
Warsaw (Poland), September 17-20 2018.

25. *Computational Quantum Materials*
International conference on modeling and simulations of emerging materials;
Abbottabad University (Pakistan), July 2-4 2018.

24. *Tunable quantum-phases in spin-orbit oxides*
    7th International Symposium on Structure-Property Relationships in Solid State Materials;
    Montesilvano-Pescara (Italy), June 8-13 2018.

23. *Correlation effects and magnetism in relativistic oxides*
    CIMTEC 2018 - 14th International Ceramics Congress & 8th Forum on New Materials;
    Perugia (Italy), June 4-20 2018.

22. *Ab initio modelling beyond DFT*
    SNRC Colloqium;
    Spanish National Research Council, Madrid (Spain), November 2017.

21. *Computational Materials Modelling by First Principles*
    Workshop on Materials Modeling and Simulations;
    Abbottabad University (Pakistan), February 2017.

20. *Collective effects in relativistic oxides*
    CECAM workshop: Computational methods towards engineering novel correlated materials;
    Lausanne (Switzerland), October 2016.

19. *Polaron-driven (1×2)-reconstruction of rutile TiO_2(110)*
    Annual meeting of the Austrian Physical Society;
    Vienna (Austria), September 2016.

18. *Hybrid functionals for simulating complex oxides*
    APS March Meeting Meeting;
    Baltimora (USA), March 2016.

17. *Excess electrons and holes in oxides*
    University of Modena;
    Modena (Italy), October 2015.

16. *Electronic Structure of Perovskites: Lessons from Hybrid Functionals*
    Autumn School on Correlated Electrons: Many-Body Physics: From Kondo to Hubbard;
    Jülich (Germany), September 2015.

15. *Small and Large Polarons in TiO2 Rutile and Anatase surfaces*
    1st International Conference on Computational Design and Simulation of Materials;
    Shenyang (China), August 2015.

14. *Orbital-Lattice-Spin Interactions in Functional Materials*
    University of Pavia;
    Pavia (Italy), April 2015.

13. *Small and Large Polarons in TiO2 Rutile and Anatase surfaces*
    MRS Fall Meeting;
    Boston (USA), December 2014.

12. *Perovskites for oxide electronics and photovoltaic applications*
International Conference of Young Researchers on Advances Materials;
Haikou (China), October 2014.

11. *Electron-Lattice Interaction and Electronic Correlation in $BaBiO_3$*
CECAM Workshop (Towards) Room Temperature Superconductivity;
Lorentz Center, Leiden (Netherlands), July 2014.

10. *Electron localization in anatase and rutile TiO_2* Collaborative Conference on Crystal Growth;
Cancun (Mexico), June 2013.

9. *Screened Hybrid functionals applied to 3d-4d-5d compounds*
International Conference on Advances Materials Modelling;
Nantes (France), June 2012.

8. *Screened hybrid density functionals applied to 3d, 4d, and 5d transition metal perovskites*
Joint European Magnetic Symposia;
Parma (Italy), June 2012.

7. *Hybrid Functionals and GW for oxides: a beyond-DFT perspective*
CECAM Workshop;
Zaragoza (Spain), June 2011.

6. *Post-DFT methods for complex oxides*
Shenyang National Laboratory for Materials Science;
Shenyang (China), February 2011.

5. *Small polarons in semiconductors by hybrid functionals*
Young International Scientist Fellowship, award ceremony, Chinese Academy of Sciences;
Shenyang (China), October 2010.

4. *Multivalency and polaronic hole trapping in $BaBiO_3$*
University of California Santa Barbara;
Santa Barbara (USA), March 2010.

3. *Multivalency and polaronic hole trapping in $BaBiO_3$*
APS March Meeting;
Portland (USA), March 2010.

2. *Magnetism in transition metal oxides by post-DFT methods*
Psi-k Workshop on Magnetism in Complex Systems;
Vienna (Austria), April 2009.

1. *DFT for superconductors*
Talk @ Institute of Physical Chemistry, University of Vienna;
Vienna (Austria), May 2005.

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