Jan Kuneš

Date of birth:	May 27, 1974
Nationality:	Czechia
Office address:	Institute of Solid State Physics TU Wien Wiedner Hauptstr. 8 1040 Wien Austria

Areas of Research

- Condensed matter theory with focus on real materials
- Electronic correlations and magnetism
- Theory of photoemission, optical and magneto-optical spectroscopies
- Numerical many-body methods
- Density functional methods for solids

Education

1997	**M.Sc.** in Physics at the Faculty of Mathematics and Physics, Charles University, Prague with thesis: "*Vortex dynamics in $Bi_2Sr_2CaCu_2O_8$ single-crystals*" Advisor: Dr. Zdeněk Janu
2002	**Ph.D.** in Physics at the Faculty of Mathematics and Physics, Charles University, Prague with thesis: "*Ab initio calculations of magneto-optical effects in magnetics*" Advisor: Dr. Pavel Novák

Scientific Career

09/1998 – 08/2002	Doctoral student, Institute of Physics, Czech Academy of Sciences, Prague (Czechia)
09/2002 – 09/2005	Postdoctoral research associate, University of California, Davis (USA)
01/2006 – 06/2007	Alexander von Humboldt Research Fellow, Center for Electronic Correlations and Magnetism, University of Augsburg (Germany)
07/2007 – 12/2009	Research associate, Center for Electronic Correlations and Magnetism, University of Augsburg (Germany)
01/2010 –	Senior staff scientist, Institute of Physics, Czech Academy of Sciences, Prague (Czechia)
09/2016 – 08/2017	Assistant Professor, TU Wien (Austria)

09/2017– Associate Professor (permanent), TU Wien (Austria)

Research Visits (> 1 month)

10/1999 – 07/2002	IFW Dresden (several stays of 12 months in total)
09/2007 – 10/2007	University of California, Davis (6 weeks)
10/2007, 02/2010	KITP Santa Barbara (2 month)
11/2008	University of Tokyo (1 month)
04/2012	Ã‰cole Polytechnique, Paris (1 month)
06/2010 – 06/2016	University of Augsburg (several stays of 5 months in total)

Service to the Community

- Head of the Ψ-k working group on Non-perturbative many-body methods (2018 –)
- Editorial board member Journal of Physics: Condensed Matter (2017– 2018)
- Member of the Ψ-k working group on Dynamical mean-field methods (2012–2017)
- Reviewer for Physical Review B, Physical Review Letters, Nature Physics, Nature Communications, Advanced Materials, Europhysics Letters, Computer Physics Communications, New Journal of Physics, Science Advances, Physica B
- Grant reviewer for Czech Science Foundation, Dept. of Energy (USA), Marsden Fund (New Zealand), TU Wien (Austria), National Science Centre (Poland), Austrian Science Fund, German Research Foundation
- External examiner: P. Thunström, (Ph.D., Uppsala University, 2012), K. Dymkowski (M.Sc., Trinity College Dublin, 2013), K. Steiner (Ph.D., University of Fribourg, 2017), R. Mondal (Ph.D., Uppsala University, 2017)

Administrative Experience

- Head of the *Spectroscopy of Magnetic Oxides* group, Department of Magnetics and Superconductors, Institute of Physics, Czech Academy of Sciences, Prague (2010-2015)
- Preparation of tender for LUNA computer cluster ($\sim$ 220.000 EUR), Institute of Physics, Czech Academy of Sciences, Prague (2013)
- Preparation of tender and a member of the selection committee for EXMAG computer cluster ($\sim$ 140.000 EUR), Institute of Physics, Czech Academy of Science, Prague (2016)
- Substitute member of the study committee "Computational Science and Egineering", TU Wien, (2018-)

Third Party Funding

01/2010-12/2012 *Magnetic and transport properties of $LaCoO_3$: Dynamical mean-field study*, Czech Science Foundation ($\sim$43.000 EUR)

08/2010-07/2013	*LDA+DMFT approach to multi-band correlation phenomena: Susceptibilities and structural relaxation*, Project P2 of DFG Research Unit 1346 (together with M. Kollar and D. Vollhardt), DFG Germany (∼318.000 EUR)
01/2013-12/2015	*Strong electron correlations in systems with spin-orbit coupling*, Czech Science Foundation (∼78.000 EUR)
08/2013-07/2016	*LDA+DMFT approach to multi-band correlation phenomena*, Project P2 of DFG Research Unit 1346 (together with M. Kollar and D. Vollhardt), DFG Germany (∼280.000 EUR)
06/2015-05/2020	*Excitonic Magnetism in Strongly Correlated Materials*, ERC Consolidator grant (1.382.000 EUR)
01/2021-12/2024	*Quantum phase transitions and collective modes*, (together with S. Bühler-Paschen, K. Held and A. Toschi) FWF Austria (703.000 EUR)

Teaching Experience

Courses

Electronic Theory of the Solid State, Prague	2016S
Computational Materials Science, TU Wien	2016W, 2018W, 2020W, 2021W
Basics of Physics II (in German), TU Wien	2018S, 2019S, 2020S, 2021S
Solid State Physics II, TU Wien	2018W, 2019W, 2020W, 2021W
Concepts in Condensed Matter Physics, TU Wien	2020W, 2021W

Lecturer at Summer Schools

06/2003	Magnetism and Magneto-optics in Density Functional Theory, *EXCITING Summer School*, Riksgransen, Sweden
10/2011	Wannier Functions and Construction of Model Hamiltonians, *Autumn School 2011: Hands-On Course on LDA+DMFT*, JÃ¼lich, Germany (not participated, published lecture notes)
09/2012, 07/2018	Wannier Function Projection, *Summer School: Bandstructure meets Many Body Theory*, Vienna, Austria

Supervision of Students and Postdocs

Undergraduate students

- Karel Pajskr, Charles University, Prague (2015 - 2016)
- Mathias Winder, TU Wien (MSc 2018)
- Dominik Huber, TU Wien (MSc 2021)

Doctoral students

- Kyo-Hoon Ahn, Korea University, Sejong (co-supervising, PhD 2018)
- Dominque Geffroy, Masaryk University, Brno (co-supervising, PhD 2017)
- Juan Fernández Afonso, Charles University, Prague & TU Wien (2015 -)
- Abuduaini Niyzai, TU Wien (2017 -)
- Mathias Winder, TU Wien (PhD 2020)

Postdocs

- Vlastimil Křápek, Institute of Physics, Czech Academy of Science, Prague (2011-2012)
- Pavel Augustinský, University of Augsburg & Institute of Physics, Czech Academy of Sciences, Prague (2012-2014)
- Vladislav Pokorný, University of Augsburg & Institute of Physics, Czech Academy of Sciences, Prague (2014-2015)
- Andrii Sotnikov, Institute of Physics, Czech Academy of Sciences, Prague & TU Wien (2015-2019)
- Atsushi Hariki, Institute of Physics, Czech Academy of Sciences, Prague & TU Wien (2016-2020)
- Dominique Geffroy, TU Wien (2017-2020)
- Kyo-Hoon Ahn, TU Wien (2019 - 2020)

Scientometry

ResearcherID: B-4484-2008

articles in refereed journals:	109
conference proceedings:	10
book chapters:	2
citations (WoS without self-citations):	∼5700
h-index (WoS):	40
invited talks at conferences (seminars):	44 (58)

Awards and Fellowships

- *Annual Prize of Bolzano Foundation*, Charles University, Czechia (2002)
- *NATO-NSF Research Fellowship*, National Science Foundation, USA (2002)
- *Humboldt Research Fellowship*, Alexander von Humboldt Foundation, Germany (2005)
- *J. E. Purkyně Fellowship*, Czech Academy of Sciences, Czechia (2008)
- *APS Outstanding Referee*, American Physical Society, USA (2015)
- *ERC Consolidator Grant*, EU (2015)

Language Skills

Czech	native
English	full professional proficiency
German	limited working proficiency

Selected publications

D. Geffroy, J. Kaufmann, A. Hariki, P. Gunacker, A. Hausoel and J. Kuneš,
Collective modes in ordered Mott systems: dynamical mean-field study
Phys. Rev. Lett. **122**, 127601 (2019).
In this paper we use the dynamical mean-field theory (DMFT), for the first time to the best of our knowledge, to study the behavior of collective excitations across a second order phase transition. We show that DMFT correctly describes the linear Goldstone modes predicted by symmetry analysis. We observe and explain the crossover from amplitude to phase fluctuations in systems with weakly broken symmetry. We provide a prediction how to identify exitonic magnet using dynamical spin structure factor.

J. Kuneš and P. Augustinský,
Excitonic condensation of strongly correlated electrons: The case of $Pr_{0.5}Ca_{0.5}CoO_3$.
Phys. Rev. B **90**, 235112 (2014).
Based on a combination of model and material specific calculations we have proposed excitonic magnetism to be realized in praseodymium cobaltites. This work since inspired several experimental and theoretical studies that supported our proposal. A conclusive proof is, nevertheless, still missing. Facilitated by the newly developed impurity solver with off-diagonal bath, we have realized orbital off-diagonal phases that were not previously studied in the Hubbard model. We have shown that excitonic condensate can be obtained also in density functional calculations for cobaltites and thus pointed out the possibility of this rather unusual order to the band structure community.

J. Kuneš and V. Křápek,
Disproportionation and Metallization at Low-Spin to High-Spin Transition in Multiorbital Mott Systems
Phys. Rev. Lett. **106**, 256401 (2011).
We have discovered spin-state ordered phase in the phase diagram of two-orbital Hubbard model. This study showed that systems close to spin-state transition exhibit unusual instabilities. This work motivated further studies into this topic, which uncovered other competing instabilities such as excitonic condensation or superconductivity. Spin-state ordered phases were since realized in more realistic LDA+DMFT calculations in $LaCoO_3$ and other materials. Attempts to find spin-state order experimentally in nature is an ongoing effort.

J. Kuneš, A. V. Lukoyanov, V. I. Anisimov, R. T. Scalettar, and W. E. Pickett,
Collapse of magnetic moment drives Mott transition in MnO,
Nat. Mater. **7**, 198 (2008).
We have presented a comprehensive theory of pressure induced spin-state crossover in MnO using the density functional plus dynamical mean-field theory (LDA+DMFT). We have explained the connection between the spin-state crossover, metal-insulator transition and volume collapse in this prototype material. This work was among early demonstrations the DMFT capabilities for real materials in a situation where different conventional density functionals (LDA vs LDA+U) were necessary to provide at least approximate descriptions of the low- and

high-pressure phases.

J. Kuneš, R. Arita, P. Wissgott, A. Toschi, H. Ikeda, K. Held,
Wien2wannier: From linearized augmented plane waves to maximally localized Wannier functions,
Comput. Phys. Commun. **181**, 1888 (2010). We have used detailed knowledge of the Wien2k package for band structure calculations to implement an interface to the wannier90 code for construction of Wannier functions. While this is a purely technical development it has been widely used by the community since then and allowed us as well as many other to construct material specific models in an unbiased way.

List of publications

121. D. Takegami, C. Y. Kuo, K. Kasebayashi, J.-G. Kim, C. F. Chang, C. E. Liu, C. N. Wu, D. Kasinathan, S. G. Altendorf, K. Hoefer, F. Meneghin, A. Marino, Y. F. Liao, K. D. Tsuei, C. T. Chen, K.-T. Ko, A. GÃ¼nther, S. G. Ebbinghaus, J. W. Seo, D. H. Lee, G. Ryu, A. C. Komarek, S. Sugano, Y. Shimakawa, A. Tanaka, T. Mizokawa, J. Kuneš, L. H. Tjeng, and A. Hariki,
$CaCu_3Ru_4O_{12}$: a high Kondo-temperature transition metal oxide
Phys. Rev. X **12**, *011017 (2022).*

120. A. Hariki, K.-H.Ahn and J. Kuneš,
Valence skipping, internal doping and site-selective Mott transition in $PbCoO_3$ under pressure
Phys. Rev. B **104**, 235101 (2021).

119. K. Higashi, M. Winder, J. Kuneš, and A. Hariki,
Core-level x-ray spectroscopy of infinite-layer nickelate: LDA+DMFT study
Phys. Rev. X **11**, *041009 (2021).*

118. A. Niyazi, D. Geffroy and J. Kuneš,
Antiferromagnetic magnons and local anisotropy: dynamical mean-field study
Phys. Rev. B **104**, 075152 (2021).

117. J. Ebad-Allah, S. Rojewski, M. VÃ¶st, G. Eickerling, W. Scherer, E. Uykur, Raman Sankar, L. Varrassi, C. Franchini, K.-H. Ahn, J. Kuneš, and C. Kuntscher,
Pressure-Induced Excitations in the Out-of-Plane Optical Response of the Nodal-Line Semimetal ZrSiS
Phys. Rev. Lett. **127**, *076402 (2021).*

116. A. Niyazi, D. Geffroy and J. Kuneš,
Dynamical response and competing orders in two-band Hubbard model
Phys. Rev. B **102**, 085159 (2020).

115. M. Winder, A. Hariki and J. Kuneš,
X-ray spectroscopy of rare-earth nickelate $LuNiO_3$: LDA+DMFT study
Phys. Rev. B **102**, *085155 (2020).*

114. A. Hariki, R.-P. Wang, A. Sotnikov, K. Tomiyasu, D. Betto, N. B. Brookes, Y. Uemura, M. Ghiasi, F. M.'F. de Groot, and J. Kune

113. A. Sotnikov, K.-H. Ahn and J. Kuneš,
Ferromagnetism of $LaCoO_3$ films
SciPost Phys. **8**, 082 (2020).

112. A. Hariki, M. Winder, T. Uozumi, and J. Kuneš,
LDA+DMFT approach to resonant inelastic x-ray scattering in correlated materials
Phys. Rev. B **101**, *115130 (2020).*

111. *H. Shinaoka, D. Geffroy, M. Wallerberger, J. Otsuki, K. Yoshimi, E. Gull, and J. Kuneš,*
Sparse sampling and tensor network representation of two-particle Green's functions
SciPost Phys. **8**, 012 (2020).

110. M. Ghiasi, A. Hariki, M. Winder, J. KuneÅ¡, A. Regoutz, T.-L. Lee, Y. Hu, J.-P. Rueff, and F. M. F. de Groot,
Charge-transfer effect in hard x-ray 1s and 2p photoemission spectra: LDA+DMFT and cluster-model analysis
Phys. Rev. B **100***, 075146 (2019).*

109. *J. Fernández Afonso, A. Sotnikov, A. Hariki, and J. Kuneš,*
Pressure-induced spin-state ordering in Sr_2CoO_3F
Phys. Rev. B **99***, 205118 (2019).*

108. *K.-H. Ahn, A. Hariki, K.-W. Lee, and J. Kuneš,*
Antiferromagnetism in RuO_2 as d-wave Pomeranchuk instability
Phys. Rev. B **99***, 184432 (2019).*

107. *J. Ebad-Allah, J. FernÃ¡ndez Afonso, M. KrottenmÃ¼ller, J. Hu, Y. L. Zhu, Z. Mao, J. Kuneš and C. A. Kuntscher,*
Chemical pressure effect on the optical conductivity of the nodal-line semimetals ZrSiY (Y=S, Se, Te) and ZrGeY (Y=S, Te)
Phys. Rev. B **99***, 125154 (2019).*

106. *D. Geffroy, J. Kaufmann, A. Hariki, P. Gunacker, A. Hausoel and J. Kuneš,*
Collective modes in ordered excitonic magnets: dynamical mean-field study
Phys. Rev. Lett. **122***, 127601 (2019).*

105. *Z. Huesges, K. Kliemt, C. Krellner, R. Sarkar, H-H. KlauÃŸ, C. Geibel, M. Rotter, P. Novák, J. Kuneš and O. Stockert,*
Analysis of the crystal electric field parameters of $YbNi_4P_2$
New J. Phys. **20***, 073021 (2018).*

104. *A. Hariki, M. Winder and J. Kuneš,*
Continuum Charge Excitations in High-Valence Transition-Metal Oxides Revealed by Resonant Inelastic X-Ray Scattering
Phys. Rev. Lett. **121***, 126403 (2018).*

103. *R.-P. Wang, A. Hariki, A. Sotnikov, F. Frati, J. Okamoto, H.-Y. Huang, A. Singh, D.-J. Huang, K. Tomiyasu, C.-H. Du, J. Kuneš and F. M. F. de Groot,*
Excitonic dispersion of the intermediate-spin state in $LaCoO_3$ revealed by resonant inelastic X-ray scattering
Phys. Rev. B **90***, 035149 (2018).*

102. *A. Sotnikov, A. Cichy and J. Kuneš,*
Suppression and revival of long-range ferromagnetic order in the multiorbital Fermi-Hubbard model
Phys. Rev. B **97***, 235157 (2018).*

101. *D. Geffroy, A. Hariki and J. Kuneš,*
Excitonic magnet in external field: complex order parameter and spin currents
Phys. Rev. B **97**, *155114 (2018).*

100. *J. Fernandez Afonso, A. Sotnikov and J. Kuneš,*
Theoretical investigation of excitonic magnetism in $LaSrCoO_4$
J. Phys.: Condens. Matter **30**, *135603 (2018).*

99. *A. Sotnikov and J. Kuneš,*
Competing phases in the model of Pr-based cobaltites
Phys. Rev. B **96**, *245102 (2017).*

98. *A. Hariki, A. Hausoel, G. Sangiovanni and J. Kuneš,*
DFT+DMFT study on soft moment magnetism and covalent bonding in $SrRu_2O_6$
Phys. Rev. B **96**, *155135 (2017).*

97. *P. Wadley, K.W. Edmonds, M.R. Shahedkhah, R.P. Campion, B.L. Gallagher, J. Železný, J. Kuneš, V. Novák, T. Jungwirth, V. Saidl, P. Němec, F. Maccherozzi and S. S. Dhesi,*
Control of antiferromagnetic spin axis orientation in bilayer Fe/CuMnAs films
Sci. Rep. **7**, *11147 (2017).*

96. *A. Hariki, T. Uozumi and J. Kuneš,*
LDA+DMFT approach to core-level spectroscopy: application to 3d transition metal compounds
Phys. Rev. B **96**, *045111 (2017).*

95. *J. Kuneš, I. Leonov, P. Augustinský, V. Křápek, M. Kollar and D. Vollhardt,*
LDA+DMFT approach to ordering phenomena and the structural stability of correlated materials
Eur. Phys. J. Spec. Top. **226**, *2641 (2017).*

94. *A. Golubeva, A. Sotnikov, A. Cichy, J. Kuneš, and W. Hofstetter,*
Breaking of SU(4) symmetry and interplay between strongly-correlated phases in the Hubbard model
Phys. Rev. B **95**, *125108 (2017.)*

93. *J. Fenández Afonso and J. Kuneš,*
Excitonic magnetism in d^6 perovskites
Phys. Rev. B **95**, *115131 (2017).*

92. *K.-H. Ahn, K. Pajskr, K.-W. Lee and J. Kuneš,*
Calculated g-factors of 5d double perovskites Ba_2NaOsO_6 and Ba_2YOsO_6
Phys. Rev. B **95**, *064416 (2017).*

91. *V. Saidl, P. Němec, P. Wadley, V. Hills, R.P. Campion, V. Novák, K.W. Edmonds, F. Maccherozzi, S. S. Dhesi, B.L. Gallagher, F. Trojánek, J. Kuneš, J. Železný, P. Malý, and T. Jungwirth*

Optical determination of the Neel vector in a CuMnAs thin-film antiferromagnet
Nat. Photon. **11**, *91 (2017).*

90. *A. Sotnikov and J. Kuneš,*
Field-induced exciton condensation in $LaCoO_3$
Sci. Rep. **6**, *30510 (2016).*

89. *J. Kuneš and D. Geffroy,*
Spontaneous Spin Textures in Multiorbital Mott Systems
Phy. Rev. Lett. **116**, *256403 (2016).*

88. *P. Wadley, B. Howells, J. Železný, C. Andrews, V. Hills, R. P. Campion, V. Novak, K. Olejnik, F. Maccherozzi, S. S. Dhesi, S. Y. Martin, T. Wagner, J. Wunderlich, F. Freimuth, Y. Mokrousov, J. Kuneš, J. S. Chauhan, M. J. Grzybowski, A. W. Rushforth, K. W. Edmonds, B. L. Gallagher, and T. Jungwirth,*
Electrical switching of an antiferromagnet
Science **351**, *587 (2016).*

87. *E. Assmann, P. Wissgott, J. Kuneš, A. Toschi, P. Blaha, and K. Held,*
Woptic: optical conductivity with Wannier functions and adaptive k-mesh refinement
Comput. Phys. Commun. **202**, *1 (2016).*

86. *K. Pajskr, P. Novák, V.Pokorný, J. Kolorenč, R. Arita, and J. Kuneš,*
On the possibility of excitonic magnetism in Ir double perovskites
Phys. Rev. B **93**, *035129 (2016).*

85. *J. Kuneš,*
Excitonic condensation in systems of strongly correlated electrons
J. Phys.: Condens. Matter **27**, *333201 (2015) - Topical Review*

84. *J. Panas, A. Kauch, J. Kuneš, D. Vollhardt, and K. Byczuk,*
Numerical calculation of spectral functions of the Bose-Hubbard model using B-DMFT
Phys. Rev. B **92**, *045102 (2015).*

83. *K.-H. Ahn, K.-W. Lee and J. Kuneš,*
Doping-dependent bandwidth renormalization and spin-orbit coupling in $(Sr_{1-x}La_x)_2RhO_4$
J. Phys.: Condens. Matter **27**, *085602 (2015).*

82. *J. Kuneš,*
Phase diagram of exciton condensate in doped two-band Hubbard model
Phys. Rev. B **90**, *235140 (2014).*

81. *J. Kuneš and P. Augustinský,*
Excitonic condensation of strongly correlated electrons: The case of $Pr_{0.5}Ca_{0.5}CoO_3$.
Phys. Rev. B **90**, *235112 (2014).*

80. *P. Novák, J. Kuneš and K. Knížek,*
Crystal field of rare earth impurities in LaF_3
Optical Materials **37***, 414 (2014).*

79. *A. Bauer, A. Regnat, C. G. F. Blum, S. Gottlieb-Schónmeyer, B. Pedersen, M. Meven, S. Wurmehl, J. Kuneš, and C. Pfleiderer,*
Low-temperature properties of single-crystal CrB_2
Phys. Rev. B **90***, 064414 (2014).*

78. *J. Kuneš and P. Augustinský,*
Excitonic Instability at the Spin-State Transition in Two-Band Hubbard Model
Phys. Rev. B **89***, 115134 (2014).*

77. *X. Marti, I. Fina, C. Frontera, Jian Liu, P. Wadley, Q. He, R. J. Paull, J. D. Clarkson, J. Kudrnovský, I. Turek, J. Kuneš, D. Yi, J-H. Chu, C. T. Nelson, L. You, E. Arenholz, S. Salahuddin, J. Fontcuberta, T. Jungwirth, and R. Ramesh,*
Room-temperature antiferromagnetic memory resistor
Nat. Mater. **13***, 367 (2014).*

76. *P. Novák, K. Knížek, M. Maryško, Z. Jirák, and J. Kuneš,*
Crystal field and magnetism of Pr^{3+} and Nd^{3+} ions in orthorhombic perovskites
J. Phys.: Condens. Matter **25***, 446001 (2013).*

75. *M. Brasse, L. Chioncel, J. Kuneš, A. Bauer, A. Regnat, C. G. F. Blum, S. Wurmehl, C. Pfleiderer, M. A. Wilde, and D. Grundler,*
De Haas-van Alphen effect and Fermi surface properties of single crystal CrB_2
Phys. Rev. B **88***, 155138 (2013).*

74. *Q.Li, G. Cao, S. Okamoto, J. Yi, W. Lin, B. C. Sales, J. Yan, R. Arita, J. Kuneš, A. V. Kozhevnikov, A. G. Eguiluz, M. Imada, Z. Gai, M. Pan, and D. G. Mandrus,*
Microscopic and Spectroscopic Evidence for a Slater Metal-Insulator Transition in Sr_2IrO_4
Sci. Rep. **3***, 3073 (2013).*

73. *P. Novák, K. Knížek and J. Kuneš,*
Crystal field parameters with Wannier functions: Application to rare-earth aluminates
Phys. Rev. B **87***, 20513 (2013).*

72. *P. Augustinský, V. Křápek and J. Kuneš,*
Doping Induced Spin State Transition in $LaCoO_3$: Dynamical Mean-Field Study
Phys. Rev. Lett. **110***, 267204 (2013).*

71. *Pavel Augustinský and Jan Kuneš,*
Improved Green's Function Measurement for Hybridization Expansion Quantum Monte Carlo
Comput. Phys. Commun. **184***, 2119 (2013).*

70. *V. Křápek, P. Novák, J. Kuneš, D. Novoselov, Dm. M. Korotin, and V. I. Anisimov,*
Spin state transition and covalent bonding in $LaCoO_3$
Phys. Rev. B **86**, *195104 (2012).*

69. *P. Wissgott, J. Kuneš, A. Toschi, and K. Held,*
Dipole matrix element approach vs. Peierls approximation for the optical conductivity
Phys. Rev. B **85**, *205133 (2012).*

68. *J. Kuneš, V. Křápek, N. Parragh, G. Sangiovanni, A. Toschi, and A. V. Kozhevnikov,*
Spin state of negative charge-transfer material $SrCoO_3$
Phys. Rev. Lett. **109**, *117206 (2012).*

67. *R. Arita, J. Kuneš, A. V. Kozhevnikov, A. G. Eguiluz, and M. Imada,*
Ab initio Studies on the Interplay between Spin-Orbit Interaction and Coulomb Correlation in Sr_2IrO_4 and Ba_2IrO_4
Phys. Rev. Lett. **108**, *086403 (2012).*

66. *K. Byczuk, J. Kuneš, W. Hofstetter, and D. Vollhardt,*
Quantification of correlations in quantum many-particle systems
Phys. Rev. Lett. **108**, *087004 (2012).*

65. *J. Kuneš,*
Wannier functions in The LDA+DMFT approach to strongly correlated materials *in Lecture Notes of the Autumn School 2011 Hands-on LDA+DMFT ed. E. Pavarini, E. Koch, D. Vollhardt, and A. I.'Lichtenstein,*
Forschungszentrum Juelich GmbH Zentralbibliothek, Verlag, 2011

64. *J. Kuneš and V. I. Anisimov,*
Various scenarios of metal-insulator transition in strongly correlated materials
Ann. Phys. (Berlin) **523**, *682 (2011).*

63. *J. Kuneš and V. Křápek,*
Disproportionation and Metallization at Low-Spin to High-Spin Transition in Multiorbital Mott Systems
Phys. Rev. Lett. **106**, *256401 (2011).*

62. *J. Kuneš,*
Efficient treatment of two-particle vertices in dynamical mean-field theory
Phys. Rev. B **83**, *085102 (2011).*

61. *J. Kuneš, R. Arita, P. Wissgott, A. Toschi, H. Ikeda, K. Held,*
Wien2wannier: From linearized augmented plane waves to maximally localized Wannier functions,
Comput. Phys. Commun. **181**, *1888 (2010).*

60. *J. Kuneš, I. Leonov, M. Kollar, K. Byczuk, V. I. Anisimov, D. Vollhardt,*
Dynamical mean-field approach to materials with strong electronic correlations,
Eur. Phys. J. Special Topics **180**, *1 (2010).*

59. *H. Ikeda, R. Arita and J. Kuneš,*
Doping dependence of spin fluctuations and electron correlations in iron pnictides
Phys. Rev. B **82**, *024508 (2010).*

58. *H. Ikeda, R. Arita and J. Kuneš,*
Phase diagram and gap anisotropy in iron-pnictide superconductors,
Phys. Rev. B **81**, *054502 (2010).*

57. *J. Kuneš, L. Baldassarre, B. Schächner, K. Rabia, C. A. Kuntscher, Dm. M. Korotin, V. I. Anisimov, J. A. McLeod, E. Z. Kurmaev, and A. Moewes,*
Metal-insulator transition in $NiS_{2-x}Se_x$,
Phys. Rev. B **81**, *035112 (2010).*

56. *M. Sentef, J. Kuneš, P. Werner, and A. P. Kampf,*
Correlations in a band insulator,
Phys. Rev. B **80**, *155116 (2009).*

55. *A. Shitade, H. Katsura, J. Kuneš, X.-L. Qi, S.-C. Zhang, and N. Nagaosa,*
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45. *K.-W. Lee, J. Kuneš, R. T. Scalettar, and W. E. Pickett,*
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42. *Deepa Kasinathan, K. Koepernik, J. Kuneš, H. Rosner, W. E. Pickett,*
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41. *W. Kuch, F. Offi, L. I. Chelaru, J. Wang, K. Fukumoto, M. Kotsugi, J. Kirschner, and J. Kuneš,*
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4. *J. Kuneš and J. Mistrík,*
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3. *J. Kuneš and P. M. Oppeneer,*
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Invited Presetations

CONFERENCES

44. Superfluid, solid and supersolid in two-orbital Hubbard model
Excitonic condensation and competing orders in low-dimensional materials, CECAM workshop (online), June 2021

43. Towards predictive theory of two-particle spectroscopies in strongly correlated materials
Theory Meets Experiment in Low-Dimensional Structures with Correlated Electrons, Prague, Czechia, July 2019

42. LDA+DMFT approach to calculation of RIXS spectra
11th International Conference on Inelastic X-ray Scattering (IXS2019), Stony Brook, USA, June 2019

41. Dynamical susceptibilities and spontaneous symmetry breaking with dynamical mean-field theory
19th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods,*Trieste, Italy, January 2019*

40. Excitonic magnetism in strongly correlated materials
Excitonic insulator: New perspectives in long-range interacting systems, *Lausanne, Switzerland, September 2018*

39. Wannier function projection (wien2wannier within Wien2k)
Bandstructure meets quantum field theory, *Wien, Austria, July 2018*

38. Excitonic magnetism in models and materials
Mini-Symposium:Toward Control of Magnetic Phases in Materials, *Uppsala, Sweden, October 2017*

37. Field induced effects in excitonic magnets
3rd International Workshop on Dynamical Mean-Field Approach for Strongly Correlated Materials, *Dresden, Germany, September 2017*

36. Towards spontaneous spin-galvanic effect
Green's function methods: the next generation III, *Toulouse, France, June 2017*

35. Spectroscopic signatures of excitonic magnetism
Ab initio correlated methods in spectroscopy, *Prague, Czechia, February 2017*

34. Meta-magnetic transition in $LaCoO_3$ - a field induced exciton condensation?
Computational methods towards engineering novel correlated materials, *Lausanne, Switzerland, October 2016*

33. Spin textures in Hubbard systems
What about U?, *Trieste, Italy, October 2016*

32. *Excitonic condensation in models and materials*
Next generation quantum mateials, *Sao Paulo, Brazil, April 2016*

31. *Excitonic condensation of strongly correlated electrons*
CORPES 2015, *Paris, France, July 2015*

30. *Excitonic condensation in systems of strongly correlated electrons*
Ψ-k workshop: Strong electron correlation effects in complex d- and f-based magnetic materials for technological applications, *Prague, Czechia, July 2014*

29. *Excitonic condensation in systems of strongly correlated electrons*
What about U?, *Lausanne, Switzerland, June 2014*

28. *Spin-orbit physics of iridates with Wien2k*
Electronic properties of spin-orbit driven oxides, *Dresden, Germany, September 2013*

27. *Wannier functions: theory and selected applications*
Ab initio Dynamical vertex approximation workshop, *Baumschlagerberg, Austria, September 2013*

26. *Correlation phenomena in the vicinity of spin state transition,*
Dynamical Mean-Field Approach for Strongly Correlated Materials, *Dresden, Germany, September 2012*

25. *Thermal and doping effects in materials with competing multiplets,*
Mini 2012 - workshop on computational condensed matter physics, materials science and nanoscience from first principles, *Barcelona, Spain, January 2012*

24. *Ordering and Spatial Inhomogeneities in the Vicinity of High-Spin Low-Spin Transitions,*
Electronic Correlations in Models and Materials, *Augsburg, Germany, September 2011*

23. *Electronic Correlations in Computer: from Models to Materials,*
17th Conference of Slovak and Czech Physicists, *Zilina, Slovakia, September 2011*

22. *Multireference Local States in Solids with Dynamical Mean-Field Theory,*
Strong Correlations from First Principles, *Seeon, Gemany, August 2011*

21. *Dynamical Correlations in Transition Metal Compounds,*
Goldschmidt 2011, *Prague, Czechia, August 2011*

20. *Spin State Transitions in Strongly Correlated Systems,*
The New Generation in Strongly Correlated Electron Systems, *Santiago de Compostela, Spain, July 2011*

19. *Covalency vs Correlation: Band Insulator with Hubbard U,*
Ψ-k 2010, *Berlin, Germany, September 2010*

18. *Origin of Metal-Insulator Transition in $NiS_{2-x}Se_x$,*
QS2C Theory Forum: 2010 Topical Meeting Advanced First-Principles Calculations and Many-Body Effects in Correlated Electrons, *RIKEN, Tokyo, Japan, September 2010*

17. *Electronic Correlations in Materials with LDA+DMFT Approach,*
IUMRS-ICEM 2010*, Seoul, Korea, August 2010*

16. *From a fluctuating to an intermediate valence: Yb under pressure,*
Workshop on Recent Developments in Dynamical Mean Field Theory*, Zurich, Switzerland, September 2009*

15. *Selected Transition Metal Oxides with Dynamical Mean-Field Approximation,*
Magnetite 2009*, Prague, Czech Republic, January 2009*

14. *Correlation vs Hybridization in Transition Metal Compounds,*
Computational Material Science Network Meeting*, Oak Ridge National Laboratory, USA, November 2008*

13. *Moment Collapse and Metalization in Transition Metal Oxides,*
16th International Conference on Solid Compounds of Transition Elements*, Dresden, Germany, July 2008*

12. *Transition Metal Oxides: Mott Transition under Pressure,*
20th Annual Workshop on Recent Developments in Electronic Structure Methods*, Urbana, USA, June 2008*

11. *Collapse of Magnetic Moment Drives the Mott Transition in MnO,*
SFB484 annual meeting*, Irsee, Germany, April 2008*

10. *Magnetic Moment Collapse-Driven Mott Transition in MnO,*
March Meeting of American Physical Society*, New Orleans, LA, March 2008*

9. *Moment-Collapse Driven Mott Transition in MnO under Pressure,*
Computational Materials Science Network Meeting*, University of California Davis, CA, September 2007*

8. *KOs_2O_6: Superconducting Rattler,*
Workshop on Ab Initio Approaches to Electron Phonon Coupling and Superconductivity*, Donostia - San Sebastian, Spain, May 2007*

7. *NiO - DMFT Study of Charge-Transfer Insulator,*
Workshop on Realistic Theory of Electron Correlations*, Institute of Physics AS CR, Prague, Czech Republic, May 2007*

6. *Frustration and Lattice Dynamics in Potassium Osmate,*
M2S-HTSC Conference*, Dresden, Germany, July 2006*

5. *Charge Disproportionation in $Na_{0.5}CoO_2$Studied by LDA+U Method,*
March Meeting of American Physical Society*, Baltimore, MR, March 2006*

4. *Pyrochlore Superconductors: What is the Difference between K and Rb?,*
FPLO Workshop*, Leibniz Institute for Solid State Research, Dresden, Germany, March 2005*

3. *Ab initio calculations of magneto-optical effects,*
   MORIS 2002*, Benodet, France, May 2002*

2. *Ab Initio Calculations of Magneto-Optical Kerr Effect,*
   The 6th Prague Colloquium on f-electron Systems*, Prague, Czechia, May 2002*

1. *Relativistic Local Orbitals in Wien2k: Bulk Properties of Light Actinides,*
   FPLO Workshop*, Leibniz Institute for Solid State Research, Dresden, Germany, March 2002*

SEMINARS AND COLLOQUIA

58. LDA+DMFT approach to calculation of core-level spectra
University of Erlangen, Germany, January 2022

57. LDA+DMFT approach to calculation of core-level spectra
Ludwig-Maximilians-University, Munich, Germany, April 2021

56. Core-level spectroscopy of transition metal oxides
Institute of Applied Physics, TU WIEN, Austria, March 2021

55. Thermal damping of spinful excitons in $LaCoO_3$: theory and experiment
University of Warsaw, Poland, January 2021

54. Thermal damping of spinful excitons in $LaCoO_3$: theory and experiment
Faculty of Mathematics and Physics, Charles University, Prague, Czechia, December 2020

53. Thermal damping of spinful excitons in $LaCoO_3$: theory and experiment
University of Augsburg, Germany, July 2020

52. Towards predictive theory of two-particle spectroscopies in strongly correlated materials
Brookhaven National Laboratory, USA, June 2019

51. Excitonic Condensation of Strongly Correlated Electrons
College de France, Paris, France, May 2019

50. Exitonic magnetism in models and materials
University of Stuttgart, Germany, July 2018

49. Excitonic condensation: a route to new magnetic materials
University of Augsburg, Germany, May 2017

48. Excitonic magnetism in models and materials
University of Fribourg, Switzerland, April 2016

47. Excitonic magnetism in models and materials
TU Wien, Austria, January 2016

46. Excitonic condensation of strongly correlated electrons
TU Munich, Germany, December 2015

45. Excitonic condensation of strongly correlated electrons
European XFEL, Hamburg, Germany, December 20155

44. Excitonic condensation of strongly correlated electrons
Masaryk University, Brno, Czechia, November 2015

43. Excitonic condensation of strongly correlated electrons
TU Wien, Austria, June 2015

42. Excitonic condensation of strongly correlated electrons,
University of Duisburg, Germany, January 2015

41. Excitonic condensation of strongly correlated electrons,
Max-Planck Institute for Chemical Physics of Solids, Dresden, November 2014

40. Excitonic condensation in models and materials,
University of Augsburg, Germany, June 2014

39. Towards material specific theory of ordering phenomena: two-particle response in DMFT,
Warsaw University, Poland, November 2012

38. Electronic correlations and spin-state transitions,
Warsaw University, Poland, November 2012

37. Correlation phenomena in the vicinity of spin state transitions,
Max-Planck Institute for Solid State Research, Stuttgart, Germany, October 2012

36. Electronic correlations in the vicinity of spin state transitions,
Technical University Dresden, Germany, June 2012

35. Thermal effects in materials with competing multiplets
Ecole Polytechnique, Paris, France, April 2012

34. Surprising effects of electronic correlations in band insulators, Department of Condensed Matter Physics,
Charles University, Prague, Czechia, October 2011

33. Electronic correlations in computer: from medels to materials,
Masaryk University, Brno, Czechia, October 2011

32. Spin disproportionation at high-spin–low-spin transition in $LaCoO_3$,
University of Augsburg, Germany, May 2011

31. Towards material specific theory of ordering phenomena: two-particle response in DMFT,
University of Wuerzburg, Germany, January 2011

30. Computer simulations of electronic correlations in solids,
Institute of Physics, Prague, Czechia, October 2010

29. Electronic structure of Strongly Correlated Materials,
Sungkyunkwan University, Suwon, Korea, August 2010

28. Correlations in Models and Materials,
Sungkyunkwan University, Suwon, Korea, August 2010

27. Towards Two-Particle Response Functions in DMFT,
University of Augsburg, Germany, July 2010

26. Electronic Correlations and Covalency: Dynamical Mean-Field Perspective,
University of Mainz, Germany, June 2010

25. Strongly Correlated Materials with Dynamical Mean-Field Theory,
Fritz-Haber-Institute, Berlin, Germany, May 2010

24. Electronic Correlations in Models and Materials,
Theory seminar, Department of Condensed Matter Physics, Charles University, Prague, April 2010

23. Electronic Correlation Effects in Solids,
Department of Condensed Matter Physics, Charles University, Prague, April 2010

22. Correlations & Covalency: Dynamical Mean-Field Theory of Charge-Transfer Compounds,
University of California Davis, USA, February 2010

21. From Clusters to Crystals: Application of the Dynamical Mean-Field Theory to Materials,
CM Theory Department, Institute of Physics, AS CR, Prague, Czechia, February 2010

20. Simultaneous Spin and Metal-Insulator Transition in TM Oxides,
Ludwig-Maximilians-University Munich, Germany, June 2009

19. What Do the Correlations Do? Selected Materials with Dynamical Mean-Field Theory,
IFW Dresden, Germany, May 2009

18. Metal-Insulator Transition in $NiS_{2-x}Se_x$: Is NiS_2 a Charge-Transfer Insulator?,
ETH Zurich, Switzerland, February 2009

17. Electronic Structure of EuB_6: Insights from Optical Spectroscopy,
Vienna University of Technology, Austria, January 2009

16. Simultaneous Spin and Metal-Insulator Transition in TM Oxides,
University of Tokyo, Japan, November 2008

15. Crystal-Field Driven Mott Transition in MnO under High Pressure,
University of Cologne, Germany, May 2008

14. Dynamical Mean-Field Studies of Transition Metal Oxides,
Research Center Jülich, Germany, May 2008

13. Mott Transition in MnO under Pressure,
Institute of Theoretical Physics, University of Frankfurt, Germany, December 2007

12. The case of two late TMMO's: NiO and MnO investigated by DMFT,
Max-Planck-Institute for Solid State Research, Stuttgart, Germany, December 2007

11. Mott Transition in MnO under Pressure: Dynamical Mean-Field Study,
University of California Santa Cruz, CA, October 2007

10. Bunsenite - Hole Doping and Local Correlations in Charge Transfer Insulator,
    Brookhaven National Laboratory, NY, January 2007

9. Hole Doping and Local Correlations in a Charge Transfer Insulator,
   University of Stony Brook, NY, January 2007

8. Bunsenite - DMFT study of charge-transfer insulator,
   Ludwig-Maximilian University, Munich, Germany, November 2006

7. KOs_2O_6: a frustrated rattler,
   Ludwig-Maximilian University, Munich, Germany, June 2006

6. KOs_2O_6: a frustrated rattler,
   ETH Zurich, Switzerland, February 2006

5. KOs_2O_6: a frustrated rattler,
   University of Augsburg, Germany, January 2006

4. Lattice dynamics of KOs_2O_6,
   Oak Ridge National Laboratory, TN, March 2005

3. Exchange coupling in Europium monochalcogenides studied with LDA+U method,
   University of Augsburg, Germany, January 2005

2. Magnetism of Eu compounds,
   Max-Planck-Institute for Chemical Physics of Solid State, Dresden, Germany, January 2005

1. Calculation of magneto-optical spectra with LAPW method,
   Technical University Dresden, Germany, December 1999