

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 $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ 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	École 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 Magnetism and Superconductors, Institute of Physics, Czech Academy of Sciences, Prague (2010-2015)
- Preparation of tender for LUNA computer cluster (~ 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 (~ 140.000 EUR), Institute of Physics, Czech Academy of Science, Prague (2016)
- Substitute member of the study committee "Computational Science and Engineering", TU Wien, (2018-)

Third Party Funding

01/2010-12/2012	<i>Magnetic and transport properties of LaCoO₃: Dynamical mean-field study</i> , Czech Science Foundation (~43.000 EUR)
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08/2010-07/2013	<i>LDA+DMFT approach to multi-band correlation phenomena: Susceptibilities and structural relaxation</i> , Project P2 of DFG Research Unit 1346 (together with M. Kollar and D. Vollhardt), German Research Foundation (~318.000 EUR)
01/2013-12/2015	<i>Strong electron correlations in systems with spin-orbit coupling</i> , Czech Science Foundation (~78.000 EUR)
08/2013-07/2016	<i>LDA+DMFT approach to multi-band correlation phenomena</i> , Project P2 of DFG Research Unit 1346 (together with M. Kollar and D. Vollhardt), German Research Foundation (~280.000 EUR)
06/2015-05/2020	<i>Excitonic Magnetism in Strongly Correlated Materials</i> , ERC Consolidator grant (1.382.000 EUR)

Teaching Experience

Courses

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

Lecturer at Summer Schools

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

Supervision of Students and Postdocs

Undergraduate and project students

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

Doctoral students

- Kyo-Hoon Ahn, Korea University, Sejong (co-supervising, PhD 2018)
- Dominique 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 (2018 -)

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-)
- Dominique Geffroy, TU Wien (2017-)
- Kyo-Hoon Ahn, TU Wien (2019 -)

Scientometry

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 excitonic magnet using dynamical spin structure factor.

J. Kuneš and P. Augustinský,
Excitonic condensation of strongly correlated electrons: The case of $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{CoO}_3$.
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

109. Juan Fernández Afonso, Andrii Sotnikov, Atsushi Hariki, and Jan Kuneš,
Pressure-induced spin-state ordering in Sr_2CoO_3F
Phys. Rev. B **99**, 205118 (2019).
108. Kyo-Hoon Ahn, Atsushi Hariki, Kwan-Woo Lee, and Jan Kuneš,
Antiferromagnetism in RuO_2 as d -wave Pomeranchuk instability
Phys. Rev. B **99**, 184432 (2019).
107. J. Ebad-Allah, J. Fernández Afonso, M. Krottenmüller, 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. Klauß, 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 SrRu₂O₆
Phys. Rev. B **96**, 155135 (2017).
97. P. Wadley, K.W. Edmonds, M.R. Shahedkhah, R.P. Champion, 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. Krápek, 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 d⁶ 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 Ba₂NaOsO₆ and Ba₂YO₆
Phys. Rev. B **95**, 064416 (2017).
91. V. Saidl, P. Němec, P. Wadley, V. Hills, R.P. Champion, 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 LaCoO₃
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 $(\text{Sr}_{1-x}\text{La}_x)_2\text{RhO}_4$
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 $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{CoO}_3$.
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. Jiráček, 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 SrCoO₃* 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 Sr₂IrO₄ and Ba₂IrO₄* 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, *Quantum spin Hall effect in a transition metal oxide Na_2IrO_3* , Phys. Rev. Lett. **102**, 256403 (2009).
54. E. R. Ylvisaker, J. Kuneš, A. K. McMahan, and W. E. Pickett, *Charge Fluctuations and the Valence Transition in Yb under Pressure*, Phys. Rev. Lett. **102**, 246401 (2009).
53. J. Kuneš, Dm. M. Korotin, M. A. Korotin, V. I. Anisimov, and P. Werner, *Pressure-Driven Metal-Insulator Transition in Hematite from Dynamical Mean-Field Theory*, Phys. Rev. Lett. **102**, 146402 (2009).
52. V. I. Anisimov, Dm. M. Korotin, S. V. Streltsov, A. V. Kozhevnikov, J. Kuneš, A. O. Shorikov, and M. A. Korotin, *Density-Functional Calculation of the Coulomb Repulsion and Correlation Strength in Superconducting $LaFeAsO$* JETP Letters **88**, 729 (2008).
51. V. I. Anisimov, Dm. M. Korotin, M. A. Korotin, A. V. Kozhevnikov, J. Kuneš, A. O. Shorikov, S. L. Skornyakov, and S V. Streltsov, *Coulomb repulsion and correlation strength in $LaFeAsO$ from Density Functional and Dynamical Mean-Field Theories*, J. Phys.: Condens. Matter **21** 075602 (2009).
50. Jungho Kim, Young-June Kim, J. Kuneš, B. K. Cho, and E. J. Choi, *Optical spectroscopy and electronic band structure of ferromagnetic EuB_6* , Phys. Rev. B **78**, 165120 (2008).
49. J. Kuneš and V. I. Anisimov, *Temperature dependent correlations in covalent insulators: Dynamical mean-field approximation*, Phys. Rev. B **78**, 033109 (2008).
48. F. Tran, J. Kuneš, P. Novák, P. Blaha, L. D. Marks, and K. Schwarz, *Force calculation for orbital-dependent potentials with FP-(L)APW+lo basis set*, Comput. Phys. Commun. **179**, 784 (2008).

47. E. Z. Kurmaev, R. G. Wilks, A. Moewes, L. D. Finkelstein, S. N. Shamin, J. Kuneš, *Oxygen x-ray emission and absorption spectra as a probe of the electronic structure of strongly correlated oxides*, Phys. Rev. B **77**, 165127 (2008).
46. 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).
45. K.-W. Lee, J. Kuneš, R. T. Scalettar, and W. E. Pickett, *Correlation Effects in the Triangular Lattice Single-band System Li_xNbO_2* , Phys. Rev. B **76**, 144513 (2007).
44. J. Kuneš, V. I. Anisimov, S. L. Skornyakov, A. V. Lukoyanov, and D. Vollhardt, *NiO: Correlated Bandstructure of a Charge-Transfer Insulator*, Phys. Rev. Lett. **99**, 156404 (2007).
43. V. I. Anisimov, A. O. Shorikov, and J. Kuneš, *Magnetic state and electronic structure of plutonium from “first principles” calculations*, J. Alloys Compd. **444-445**, 42 (2007).
42. Deepa Kasinathan, K. Koepnik, J. Kuneš, H. Rosner, W. E. Pickett, *Origin of Strong Coupling in Lithium under Pressure*, Physica C **460-462**, 133 (2007).
41. W. Kuch, F. Offi, L. I. Chelaru, J. Wang, K. Fukumoto, M. Kotsugi, J. Kirschner, and J. Kuneš, *Huge magneto-crystalline anisotropy of x-ray linear dichroism observed on Co/FeMn bilayers*, Phys. Rev. B **75**, 224406 (2007).
40. J. Kuneš, V. I. Anisimov, A. V. Lukoyanov, and D. Vollhardt, *Local correlations and hole doping in NiO: A computational study*, Phys. Rev. B **75**, 165115 (2007).
39. Deepa Kasinathan, J. Kuneš, K. Koepnik, C. V. Diaconu, R. L. Martin, I. Prodan, G. E. Scuseria, N. Spaldin, L. Petit, T. C. Schulthess, and W. E. Pickett, *Mott Transition of MnO under Pressure: Comparison of Correlated Band Theories*, Phys. Rev. B **74**, 195110 (2006).
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 2. J. Kuneš and P. Novák,
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Invited Presetations

CONFERENCES

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 materials, 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, Seon, Germany, 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 $\text{NiS}_{2-x}\text{Se}_x$,
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 $\text{Na}_{0.5}\text{CoO}_2$ Studied by LDA+U Method,
March Meeting of American Physical Society, Baltimore, MD, 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

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. Excitonic 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 2015
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 models 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 $\text{NiS}_{2-x}\text{Se}_x$: 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