

Dr. Jan Kuneš

Date of birth: May 27, 1974
Office address: Institute of Physics
Academy of Sciences of the Czech Republic
Cukrovarnicka 10
16253 Praha 6, Czech Republic

Areas of Research

- Electronic correlations and magnetism
- Electronic structure of correlated electron materials
- Bandstructure calculations with density functional methods
- Optical and magneto-optical spectroscopies
- Development of new numerical tools

Scientific Career

1992 – 1997 Study of Physics, Charles University, Prague
1997 Diploma Degree in Physics, Charles University, Prague
1998 – 2002 Junior Research Fellow, Institute of Physics Academy of Sciences of the Czech Republic, Prague
2002 Ph.D. Degree in Physics, Charles University, Prague
2002 – 2005 Postdoctoral Research Associate, University of California, Davis
2006 – 2007 Alexander von Humboldt Research Fellow, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg
2007 – 2009 Research Associate, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg
2010 – Senior Scientist, Institute for Physics, Academy of Sciences of the Czech Republic

Fellowships, awards and services to the community

2002 Prize of Bolzano Foundation, Charles University, Prague
2002 NATO-NSF Research Fellowship
2006 Alexander von Humboldt Research Fellowship
2008 Fellowship J. E. Purkyně of the Czech Academy of Sciences
reviewer Phys. Rev. B, Phys. Rev. Lett., Adv. Materials, Eur. Phys. Lett., Comput. Phys. Commun.
grant reviews Grant Agency (Czech Republic), Dept. of Energy (US), Marsden Fund (New Zealand), TU Wien (Austria)

Received grants

- 2009 *Magnetic and transport properties of LaCoO₃: Dynamical mean-field study*,
Grant Agency of the Czech Republic
- 2010 *LDA+DMFT approach to multi-band correlation phenomena:
Susceptibilities and structural relaxation*, DFG Research Unit 1346,
Germany (together with M. Kollar and D. Vollhardt)

List of publications

- 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).
- 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).
- H. Ikeda, R. Arita and J. Kuneš,
Phase diagram and gap anisotropy in iron-pnictide superconductors,
Phys. Rev. B **81**, 054502 (2010).
- 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).
- M. Sentef, J. Kuneš, P. Werner, and A. P. Kampf,
Correlations in a band insulator,
Phys. Rev. B **80**, 155116 (2009).
- 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).
- 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).
- 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).
- 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).
- 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).

- J. Kuneš and V. I. Anisimov,
Temperature dependent correlations in covalent insulators: Dynamical mean-field approximation,
Phys. Rev. B **78**, 033109 (2008).
- 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).
- 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).
- J. Kuneš, A. V. Lukoyanov, V. I. Anisimov, R. T. Scalettar, and W. E. Pickett,
Collapse of magnetic moment drives Mott transition in MnO,
Nature Materials **7**, 198 (2008).
- 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).
- 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).
- 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).
- Deepa Kasinathan, K. Koepf, J. Kuneš, H. Rosner, W. E. Pickett,
Origin of Strong Coupling in Lithium under Pressure,
Physica C **460-462**, 133 (2007).
- 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).
- 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).
- Deepa Kasinathan, J. Kuneš, K. Koepf, 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).

- J. Kuneš and W. E. Pickett,
Frustration in the Coupled Rattler System KOs_2O_6 ,
Phys. Rev. B **74**, 094302 (2006).
- J. Kuneš and W. E. Pickett,
Effective Hamiltonian for potassium dynamics in the pyrochlore superconductor KOs_2O_6 ,
phys. stat.sol. (a) **203**, 2962 (2006).
- P. Schattschneider, S. Rubino, C. Hebert, J. Ruzs, J. Kuneš, P. Novák, E. Carlino,
M. Fabrizioli, G. Panaccione, and G. Rossi,
Detection of magnetic circular dichroism using a transmission electron microscope,
Nature **441**, 486 (2006).
- J. Kuneš and W. E. Pickett,
 KOs_2O_6 : superconducting rattler,
Physica B: Condensed Matter **378-380**, 898 (2006).
- P. Novák, J. Kuneš, L. Chaput, and W. E. Pickett,
Exact exchange for correlated electrons,
phys. stat. sol. (b) **243**, 563 (2006).
- D. Kashinathan, J. Kuneš, A. Lazicky, H. Rosner, C. S. Yoo, R. T. Scalettar, and W. E. Pickett,
Superconductivity and Lattice Instability in Compressed Lithium from Fermi Surface Hot Spots,
Phys. Rev. Lett. **96**, 047004 (2006).
- J. Kuneš, W. Ku, and W. E. Pickett,
Exchange Coupling in Eu Monochalcogenides from First Principles,
J. Phys. Soc. Japan **74**, 1408 (2005).
- J. Kuneš and W. E. Pickett,
Exchange coupling in Eu compounds,
Physica B: Condensed Matter **359-361**, 205 (2005).
- K.-W. Lee, J. Kuneš, P. Novák, and W. E. Pickett,
Disproportionation, metal-insulator transition, and critical interaction strength in $Na_{1/2}CoO_2$,
Phys. Rev. Lett. **94**, 026403 (2005).
- J. Kuneš, T. Jeong and W. E. Pickett
Correlation effects and structural dynamics in the beta-pyrochlore superconductor KOs_2O_6 ,
Phys. Rev. B **70**, 174510 (2004).
- J. Kuneš and R. Laskowski,
Magnetic ground state and Fermi surface of bcc Eu,
Phys. Rev. B **70**, 174415 (2004).

- K.-W. Lee, J. Kuneš, and W. E. Pickett,
Charge disproportionation and spin ordering tendencies in Na_xCoO_2 ,
Phys. Rev. B **70**, 045104 (2004).
- J. Kuneš,
Magnetism and Magneto-optics in DFT,
Physica Scripta **T109**, 166 (2004).
- J. Kuneš, P. M. Oppeneer, S. Valencia, D. Abramsohn, H.-Ch. Mertins, W. Gudat,
M. Hecker, C. M. Schneider,
*Understanding the XMLD and its magnetocrystalline anisotropy at the $L_{2,3}$ -edges of 3d
transition metals,*
J. Magn. Magn. Mater. **272-276**, 2146 (2004).
- J. Kuneš and W. E. Pickett,
Kondo and anti-Kondo coupling to local moments in EuB_6 ,
Phys. Rev. B **69**, 165111(2004).
- J. Kuneš, H. Rosner, Deepa Kasinathan, C. O. Rodriguez, and W. E. Pickett,
heory of orbital moment collapse under pressure in FeI_2 ,
Phys. Rev. B **68**, 115108 (2003).
- J. Schoenes, R. Repond, F. Hulliger, D. B. Gosh, S. K. De, J. Kuneš, and P. M. Oppeneer,
*Experimental and theoretical investigation of optical properties of dysprosium
monopnictides,*
Phys. Rev. B **68**, 085102 (2003).
- P. Novák, J. Kuneš, W. E. Pickett, Wei Ku, and F. R. Wagner,
Self-interaction correction and contact hyperfine field,
Phys. Rev. B **67**, 140403(R) (2003).
- P. M. Oppeneer, H.-Ch. Mertins, D. Abramsohn, A. Gaupp, W. Gudat, J. Kuneš, and C. M.
Schneider,
*Buried antiferromagnetic films investigated by x-ray magneto-optical reflection
spectroscopy,*
Phys. Rev. B **67**, 052401 (2003).
- J. Kuneš and P. M. Oppeneer,
*Anisotropic x-ray magnetic linear dichroism at the $L_{2,3}$ edges of cubic Fe, Co, and Ni: Ab
initio calculations and model theory,*
Phys. Rev. B **67**, 024431 (2003).
- J. Kuneš and P. M. Oppeneer,
Ab initio calculations of Magneto-optical Effects,
Trans. Magn. Soc. Jpn. **2**, 141 (2002).
- M. Kučera, J. Kuneš, A. Kolomiets, M. Diviš, A. V. Andreev, V. Sechovský, J.-P. Kappler,
and A. Rogalev,
X-ray magnetic circular dichroism studies of 5f magnetism in UCoAl and UPtAl ,
Phys. Rev. B **66**, 144405 (2002).

- J. Kuneš and V. Kamberský,
First-principles investigation of the damping of fast magnetization precession in ferromagnetic 3d metals,
Phys. Rev. B **65**, 212411 (2002).
- P. Novák, J. Kuneš, and P. M. Oppeneer,
Electronic structure of magnetite,
Physica B **312-313**, 785 (2002).
- J. Kuneš, P. Novák, P. M. Oppeneer, C. König, M. Fraune, U. Rüdiger, G. Güntherodt, and C. Ambrosch-Draxl,
Electronic structure of CrO₂ as deduced from its magneto-optical Kerr spectra,
Phys. Rev. B **65**, 165105 (2002).
- J. Kuneš, P. M. Oppeneer, H.-Ch. Mertins, F. Schafers, A. Gaupp, W. Gudat, and P. Novák,
X-ray Faraday effect of ferromagnetic films: contribution of the core exchange splitting,
J. Magn. Magn. Mater. **240**, 454 (2002).
- J. Kuneš, P. M. Oppeneer, H.-Ch. Mertins, F. Schafers, A. Gaupp, W. Gudat, and P. Novák,
X-ray Faraday effect at the L_{2,3} edges of Fe, Co, and Ni: Theory and experiment,
Phys. Rev. B **64**, 174417 (2001).
- A. V. Andreev, M. Diviš, P. Javorský, K. Prokeš, V. Sechovský, J. Kuneš, and Y. Schiokawa,
Electronic structure and magnetism in UPtAl,
Phys. Rev. B **64**, 144408 (2001).
- J. Kuneš, P. Novák, R. Schmid, P. Blaha, and J. Schwarz,
Electronic structure of fcc Th: Spin-orbit calculation with 6p_{1/2} local orbital extension,
Phys. Rev. B **64**, 153102 (2001).
- H.-Ch. Mertins, F. Schafers, A. Gaupp, W. Gudat, J. Kuneš, and P. M. Oppeneer,
Soft X-ray magnetic dichroism and Faraday rotation measured with linearly polarised light,
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- H.-Ch. Mertins, P. M. Oppeneer, J. Kuneš, A. Gaupp, D. Abramsohn, and F. Schafers,
Observation of the x-ray magneto-optical Voigt effect,
Phys. Rev. Lett. **87**, 047401 (2001).
- J. Kuneš, P. Novák, M. Diviš, and P. M. Oppeneer,
Magnetic, magneto-optical, and structural properties of URhAl from first-principles calculations,
Phys. Rev. B **63**, 20511 (2001).
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de Hass-van Alphen effect and the Fermi surface of PrNi₅,
Eur. Phys. J. B **18**, 595 (2000).

- J. Kuneš and J. Mistrík,
Magnetic, optical and magneto-optical properties of Fe-monolayer from first principles,
phys. stat. sol. (b) **220**, 991 (2000).
- J. Kuneš and P. M. Oppeneer,
Exact many-body sum rule for the magneto-optical spectrum of solids,
Phys. Rev. B **61**, 15774 (2000).
- J. Kuneš and P. Novák,
*Full-potential linearized augmented-plane-wave calculation of the magneto-optical Kerr
effect in Fe, Co and Ni,*
J. Phys.: Condens. Matter **11**, 6301 (1999).
- M. Kučera, J. Kuneš, and R. Gerber,
Magneto-optical effects of Phi^{+3} and Rh^{+4} doped yttrium iron garnet,
J. Appl. Phys. **85**, 5986 (1999).

Invited presentations

CONFERENCES

- Covalency vs Correlation: Band Insulator with Hubbard U,
Psik2010, Berlin, Germany, September 2010
- 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
- Electronic Correlations in Materials with LDA+DMFT Approach,
IUMRS-ICEM 2010, Seoul, Korea, August 2010
- From a fluctuating to an intermediate valence: Yb under pressure,
Workshop on Recent Developments in Dynamical Mean Field Theory, Zurich, Switzerland, September 2009
- Selected Transition Metal Oxides with Dynamical Mean-Field Approximation,
Magnetite 2009, Prague, Czech Republic, January 2009
- Correlation vs Hybridization in Transition Metal Compounds,
Computational Material Science Network Meeting, Oak Ridge National Laboratory, USA, November 2008
- Moment Collapse and Metalization in Transition Metal Oxides,
16th International Conference on Solid Compounds of Transition Elements, Dresden, Germany, July 2008
- Transition Metal Oxides: Mott Transition under Pressure,
20th Annual Workshop on Recent Developments in Electronic Structure Methods, Urbana, IL, June 2008
- Collapse of Magnetic Moment Drives the Mott Transition in MnO,
SFB484 annual meeting, Irsee, Germany, April 2008
- Magnetic Moment Collapse-Driven Mott Transition in MnO,
March Meeting of American Physical Society, New Orleans, LA, March 2008
- Moment-Collapse Driven Mott Transition in MnO under Pressure,
Computational Materials Science Network Meeting, University of California Davis, CA, September 2007
- KOs_2O_6 : Superconducting Rattler,
Workshop on Ab Initio Approaches to Electron Phonon Coupling and Superconductivity, Donostia - San Sebastian, Spain, May 2007
- NiO - DMFT Study of Charge-Transfer Insulator,
Workshop on Realistic Theory of Electron Correlations, Institute of Physics AS CR, Prague, Czech Republic, May 2007
- Frustration and Lattice Dynamics in Potassium Osmate,
M2S-HTSC Conference, Dresden, Germany, July 2006

- 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
- Pyrochlore Superconductors: What is the Difference between K and Rb?,
FPLO Workshop, Leibniz Institute for Solid State Research, Dresden, Germany, March 2005
- Magnetism and Magneto-optics in Density Functional Theory,
EXCITING Summer School, Riksgården, Sweden, June 2003
- Ab initio calculations of magneto-optical effects,
MORIS 2002, Benodet, France, May 2002
- Ab Initio Calculations of Magneto-Optical Kerr Effect,
The 6th Prague Colloquium on f-electron Systems, Prague, Czech Republic, May 2002
- 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

- Electronic structure of Strongly Correlated Materials,
Sungkyunkwan University, Suwon, Korea, August 2010
- Correlations in Models and Materials,
Sungkyunkwan University, Suwon, Korea, August 2010
- Towards Two-Particle Response Functions in DMFT,
University of Augsburg, Germany, July 2010
- Electronic Correlations and Covalency: Dynamical Mean-Field Perspective,
Colloquium of SFB/TRR 49, University of Mainz, Germany, June 2010
- Strongly Correlated Materials with Dynamical Mean-Field Theory,
Fritz-Haber-Institute, Berlin, Germany, May 2010
- Electronic Correlations in Models and Materials,
Theory seminar, Department of Condensed Matter Physics, Charles University, Prague,
April 2010
- Electronic Correlation Effects in Solids,
Department of Condensed Matter Physics, Charles University, Prague, April 2010
- Correlations & Covalency: Dynamical Mean-Field Theory of Charge-Transfer
Compounds,
University of California Davis, USA, February 2010
- Simultaneous Spin and Metal-Insulator Transition in TM Oxides,
Ludwig-Maximilians-University Munich, Germany, June 2009

- What Do the Correlations Do? Selected Materials with Dynamical Mean-Field Theory, IFW Dresden, Germany, May 2009
- Metal-Insulator Transition in $\text{NiS}_{2-x}\text{Se}_x$: Is NiS_2 a Charge-Transfer Insulator?, ETH Zurich, Switzerland, February 2009
- Electronic Structure of EuB_6 : Insights from Optical Spectroscopy, Technical University of Vienna, Austria, January 2009
- Simultaneous Spin and Metal-Insulator Transition in TM Oxides, University of Tokyo, Japan, November 2008
- Crystal-Field Driven Mott Transition in MnO under High Pressure, University of Cologne, Germany, May 2008
- Dynamical Mean-Field Studies of Transition Metal Oxides, Research Center Jülich, Germany, May 2008
- Mott Transition in MnO under Pressure, Institute of Theoretical Physics, University of Frankfurt, Germany, December 2007
- The case of two late TMMO's: NiO and MnO investigated by DMFT, Max-Planck-Institute for Solid State Research, Stuttgart, Germany, December 2007
- Mott Transition in MnO under Pressure: Dynamical Mean-Field Study, University of California Santa Cruz, CA, October 2007
- Bunsenite - Hole Doping and Local Correlations in Charge Transfer Insulator, Brookhaven National Laboratory, NY, January 2007
- Hole Doping and Local Correlations in a Charge Transfer Insulator, University of Stony Brook, NY, January 2007
- Bunsenite - DMFT study of charge-transfer insulator, Ludwig-Maximilian University, Munich, Germany, November 2006
- KOs_2O_6 : a frustrated rattler, Ludwig-Maximilian University, Munich, Germany, June 2006
- KOs_2O_6 : a frustrated rattler, ETH Zurich, Switzerland, February 2006
- KOs_2O_6 : a frustrated rattler, University of Augsburg, Germany, January 2006
- Lattice dynamics of KOs_2O_6 , Oak Ridge National Laboratory, TN, March 2005
- Exchange coupling in Europium monochalcogenides studied with LDA+U method, University of Augsburg, Germany, January 2005
- Magnetism of Eu compounds, Max-Planck-Institute for Chemical Physics of Solid State, Dresden, Germany, January 2005

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

