PROGRAM

ESCM2002: Electronic Structure and Computational Magnetism

Georgetown University
Washington, DC, U.S.A.

SUNDAY, JULY 14, 2002

17:00-19:00	Registration and Welcoming Reception	Physics Department

MONDAY, JULY 15, 2002

08:30-08:40	Welcome	
Session 1	**G.M. Stocks, Chair**	
08:40-09:15	G. Kotliar	Correlation Effects in Magnetic Properties: A First Principles Dynamical Mean Field Approach
09:15-09:50	R. de Groot	Spin-Injection from Half-Metals
09:50-10:10	W. Ku	Wannier State Analysis of Insulating Ferromagnetism in $La_4Ba_2Cu_2O_{10}$
10:10-10:30	**Coffee**	
Session 2	**D.D. Koelling, Chair**	
10:30-11:05	M. Troyer	Exchange Couplings in Cuprates and Vanadates from QMC and Ab-Initio Calculations
11:05-11:25	N. Kioussis	Phase Diagram of the Symmetric and Asymmetric One-dimensional Periodic Anderson Models
11:25-12:00	S.C. Erwin	Self-Compensation in Manganese-Doped Ferromagnetic Semiconductors
12:00-12:20	P. Mahadevan	Ferromagnetism in Dilute Magnetic Semiconductors
12:20-13:45	Lunch	
Session 3	**H. Eschrig, Chair**	
13:45-14:20	W. Lambrecht	Magnetic Properties of Transition Metal Impurities in SiC
14:20-14:40	Y.-J. Zhao	Advanced Tetrahedrally-Bonded Magnetic Semiconductors for Spintronic Applications
14:40-15:15	W.H. Butler	Electronic and Magnetic Structure of a Room Temperature Magnetic Semiconductor: Ilmenite-alpha-Hematite
15:15-15:35	**Coffee**	
Session 4	**D.A. Papaconstantopoulos, Chair**	
15:35-16:10	A.I. Lichtenstein	Non-Quasiparticle States in Half-Metallic Ferromagnets
16:10-16:25	I.I. Mazin	Correlated metals and the LDA+U method
16:25-17:00	P. Blaha	Charge Distribution and EFGs in Cuprates using the LDA+U Method
17:00-17:35	M.R. Pederson	2nd and 4th-order Anisotropies in Molecular Magnets
17:35-17:50	L. Senapati	Atomic Structure, Binding Energy, and Magnetic Properties of Iron Atoms Supported on Polyaromatic Hydrocarbons
18:15-21:00	**Posters and Reception**	

POSTER PAPERS

P1	A. Aguayo and D.J. Singh	Itinerant Ferromagnetism and Quantum Criticality in Sc_3In
P2	T. Baruah and M.R. Pederson	Ab initio electronic Structure and Magnetic Anisotropy Energy of Co_4-Based Single Molecule Magnet
P3	M.R. Beltran, S. Khanna, P. Jena	Determination of Magnetic Moments at the Nanoscale: The Ni_7 Case
P4	S. Cottenier, B. De Vries, J. Meersschaut, and M. Rots	The spin-density wave in Chromium: Ground State and Impurity Hyperfine Fields
P5	M. Eisenbach, B. Ujfalussy, G. Brown, and G.M. Stocks	Magnetic Properties of Iron Nanowires on Copper
P6	H.J. Gotsis and I.I. Mazin	Ferromagnetism and Spin-Orbital Compensation in Sm Intermetallics
P7	S. V. Halilov, F. Schiller, and C. Laubschat	Magnetic Surface States in Two-Dimensional Transition-Metal-Based Compounds
P8	C.S. Hellberg	Implementing Universal Quantum Computation with the Exchange Interaction
P9	M. Lach-hab, D.A. Papaconstantopoulos, I.I. Mazin and M.J. Mehl	The effect of the exchange splitting on the magnetic anisotropy of Ni
P10	P. Larson, I.I. Mazin and D.A. Papaconstantopoulos	Large Magnetic properties of YCo_5 and $SmCo_5$
P11	O. Le Bacq, A. Pasturel, A-M Dulac and S. Jobyck	Optimized Antiferromagnetic Orthophosphates for Lithium Battery Cathodes
P12	G.K.H. Madsen, K. Schwarz, P. Blaha and D.J. Singh	Magnetic Inclusion Compounds: The Alkali-Electro Sodalites and the Rare-Earth Containing Clathrates
P13	P.M. Marcus and S.L. Qiu	Instability of bcc Ferromagnetic Fe Under Pressure
P14	O.N. Mryasov and R.F. Sabirianov	A Model of Magnetization Thermal Fluctuations in Mono-Domain FePt Particles
P15	N. Noginova, E. Arthur, G. B. Loutts and V.A. Atsarkin	Slow Jahn-Teller Dynamics and Carrier Transport In Diamagnetically Diluted Perovskite Manganites
P16	D.A. Papaconstantopoulos and C.S. Hellberg	Tight-binding v. LDA+U in FeAl
P17	A. G. Petukhov and S.C. Erwin	Spin-Spin Interactions and Ferromagnetism in Mn-Doped GaAs
P18	M. Prikhodko and W. Lambrecht	Magnetic properties of Mn-N compounds
P19	D. Saifullaeva and S. Solieva	New Magnetic Semiconductors $CuCr_{1.5}Sb_{0.5}S_4$ with $CoCr_2S_4$
P20	D.J. Singh, M. Gupta and R. Gupta	Magnetism and Electronic Structure in $ZnFe_2O_4$ and $MnFe_2O_4$
P21	G. Steinle-Neumann, L. Stixrude and R. E. Cohen	Evidence for Antiferromagnetic Correlations in HCP Iron
P22	J. M. Sullivan and S. C. Erwin	Theory of the Role of Defects in Co-doped TiO_2 Anatase

TUESDAY, JULY 16, 2002

Session 5	**I.I. Mazin, Chair**	
08:30-09:05	J. Mathon	Theory of Spin-Dependant Tunneling in Magnetic Multilayers
09:05-09:40	C. Lambert	Spin-Polarised Transport in Hybrid Ferromagnetic-Superconducting Nanostructures
09:40-10:00	D. Wortmann	Spin-Polarized Ballistic Electron Transport Through an Interface by an Embedded Green-Function Approach
10:00-10:20	A. G. Petukhov	Resonant Enhancement of Tunneling Magnetoresistance in Double-Barrier Magnetic Heterostructures
10:20-10:45	M. Stiles	Transverse Spin Currents and Torques in Magnetic Multilayers
10:45-11:05	**Coffee**	
Session 6	**W.H. Butler, Chair**	
11:05-11:40	I. Mertig	Spin-Filter Effect in Metallic Nanowires
11:40-12:15	L. Nordstrom	In-Plane Uniaxial Anisotropy at the Fe/ZnSe(001) Interface
12:15-13:45	**Lunch**	
Session 7	**B.N. Harmon, Chair**	
13:45-14:20	R.W. Chantrell	Multi-Scale Modeling of Magnetic Materials
14:20-14:55	D.P. Landau	Spin Dynamics Simulations of Excitations and Critical Dynamics in a Heisenberg Antiferromagnet
14:55-15:30	G.P. Brown	Micromagnetic Modeling at Finite Temperature
15:30-15:50	P. Visscher	Spin Wave Instabilities in Magnetic Switching
15:50-16:10	**Coffee**	
Session 8	**D.J. Singh, Chair**	
16:10-16:30	V. Dobrovitski	An Approach to Multiscale Simulations of Nonlinear Magnetization Dynamics
16:30-16:45	K. Belashchenko	Multiscale approach to hysteretic phenomena: Application to CoPt-type magnets
16:45-17:20	B. Ujfalussy	Magnetic Anisotropy in Fe Multilayers on Cu
17:20-17:55	T.C. Schulthess	On the Microscopic Origin of Exchange Bias: The Role of Anisotropic Exchange
18:00-18:45	**Reception**	
18:45-21:30	**Conference Dinner**	

WEDNESDAY, JULY 17, 2002

Session 9	**A.I. Lichtenstein, Chair**	
08:30-09:05	H. Eschrig	Versions of LSDA+U for Magnetic Structures
09:05-09:40	B. Gyorffy	Exploring dynamical magnetism with Time Dependent Density Functional Theory (TDFT):from Spin Fluctuations to Gilbert Damping
09:40-10:15	J.B. Staunton	The Onset of Magnetic Order in Fe and Co Films On and Embedded in Non-Magnetic Substrates
10:15-10:35	**Coffee**	
Session 10	**J. Serene, Chair**	
10:35-10:50	S. Savrasov	Linear Response Calculations of Lattice Dynamics in Antiferromagnetic Insulators
10:50-11:25	S. Blugel	Magnetism Under the Scanning Tunneling Microscope
11:25-12:00	H. Ebert	Influence of Spin-Orbit Coupling on the Electron Spectroscopy of Non-Magnetic Metals
12:00-12:35	V.N. Antonov	Electronic Structure, Magneto-Optical Kerr Effect and X-Ray Magnetic Dichroism in Strongly Correlated Systems
12:35-13:45	**Lunch**	
Session 11	**L. Nordstrom, Chair**	
13:45-14:20	L. Sandratskii	Parameter-Free Calculation of the Exchange Interactions in Complex Magnetic Systems
14:20-14:55	M.I. Katsnelson	Many - Body Effects at Transition Metal Surfaces: an Orbital Kondo Resonance in Chromium
14:55-15:20	V.J. Thakor	Ab-initio calculations of anisotropy in spin-fluctuations of Sr_2RuO_4 and hcp-Fe
15:20-15:35	**Coffee**	
Session 12	**S. Blugel, Chair**	
15:35-16:00	R.E. Cohen	Non-Collinear Magnetism in Iron
16:00-16:20	V.P. Antropov	Self-Consistent Version of the Many Body Green Function Approach Suitable for Transition Metals Studies
16:20-16:40	O. Le Bacq	Ab-Initio Calculation of the Magnetic Anisotropy Energy of Fe-V Multilayers
16:40	**Conference Closing**	