International
Symposium and Workshop on

Electron Correlations and Materials Properties of Alloys and Compounds

Final Report

Summary

The aim of the meeting was to assess the state of the art in the study of electronic structure of materials accounting for the effects of the Coulomb interaction among the electrons in matter and to discuss applications of the novel many-body techniques for simulations of properties of *complex* materials, e.g. in the presence of structural and chemical disorder. We brought together scientists in the fields of materials simulations, and those involved in the study of strongly correlated systems. The meeting took place at Peloponnese Conference Center, AKS Hotel, Porto Heli, Greece, July 9-13, 2012. It was organized by Igor Abrikosov (Linköpings University, Sweden, e-mail: igor.abrikosov@ifm.liu.se), Nikitas Gidopoulos (Rutherford Appleton Laboratory, UK, e-mail: nikitas.gidopoulos@stfc.ac.uk), A. Gonis and P. E. A. Turchi (Lawrence Livermore National Laboratory, Livermore, CA, USA e-mails: gonis1@llnl.gov and turchi1@llnl.gov), and G. M. Stocks (Oak Ridge National Laboratory, Oak Ridge, TN USA, stocksgm@ornl.gov).

We successfully joined two conference series, International Symposium and Workshop series on Electron Correlations and Materials Properties and International Alloy Conferences, and we achieved our purpose; namely, to enhance direct contact and exchange of ideas between researchers actively working in the field of electronic structure theory of strongly correlated electron materials from across a wide spectrum of science including Condensed Matter Physics, Alloy Physics, Materials Science and Chemistry. The emphasis was the study of the effects of the Coulomb interaction – correlation effects - in affecting and shaping materials behavior across materials types, from periodic solids, compounds and alloys.

In order to enhance communication and exchange of ideas between scientists in the fields of Alloy and Materials Properties and in the formal study of Electronic Structure and Correlation Effects, the present International Workshop targeted and was opened to participants that attended the previous International Workshops as well as those that have been attending the International Alloy Conferences (IACs). Totally 58 scientists from 12 countries participated in the meeting. Importantly, the workshop attracted experienced, as well as young researchers, promoting exchange of results and ideas between them.

Among others, the workshop emphasized the following main areas:

1. New formal developments in the field of electronic structure calculations, within Density Functional Theory, Many Body Theory, Quantum Monte Carlo, as well as within other methodologies, directed at the treatment of correlation effects.
2. Electronic structure methods for excited states, including DFT.
3. Formal developments that extend to disordered systems methodologies developed for the study of correlations in periodic solids, e.g., coupling the study of correlations to the coherent potential approximation for disordered alloys.

Description of the scientific content of and discussion at the event

The format of the meeting consisted of presentations followed by discussion, a poster session, as well as a focused Discussion Sessions. The speakers were drawn from a pool of internationally acknowledged leaders in the field of electronic structure as well as junior scientists, such as post-doctoral fellows, deeply involved in current developments.

The first session of the meeting was devoted to Wave-Function-based Density Functional Theory. **Rodney Bartlett** (University of Florida) discussed Some Ruminations on Correlated Orbital Theories and the Existence of a Consistent Density Functional Theory. Contrary to conventional wisdom, a consistent density functional theory method have a functional whose total energy properties are right, and a potential whose Kohn-Sham eigenvalues are good approximations to all the principal ionization potentials in a molecule, not just the *homo*. This fact was demonstrated formally and computationally. *Ab initio DFT,* which uses elements of wave function theory mapped into KSDFT by the optimized effective potential approach, proves that such a KSDFT method with a local potential, but non-local functional can provide such a 'consistent' DFT method, contrary to all more conventional DFT approximations. Furthermore, other correlated orbital theories can be derived from purely correlated wave function considerations, potentially offering a computational alternative to DFT without its many failings. Progress toward these goals was discussed. **Andreas K. Theophilou** ("DEMOCRITOS" National Center for Scientific Research, Athens) discussed the quality of the Kohn and Sham wave functions. His point was that many exchange and correlation functionals have been proposed giving sufficient energy accuracy, although the universal one is missing. However, little work has been done on the many particle Kohn and Sham (KS) wave functions. He dealt with the spin symmetry, which was present in the exact many electron Hamiltonian, unless a nonuniform magnetic field is applied. Since the KS Hamiltonian is nonlinear it is not invariant under spin rotations and the KS states do not belong to the Irreducible representations (IrReps) of the spin symmetry, i.e. they are not eigenstates of S^2. He gave examples of such states and find their spin contamination, which was a measure of the deviation from the S^2 eigenstates. **Viktor N. Staroverov** (University of Western Ontario) discussed advances in methodology and applications of model Kohn–Sham potentials. He showed how, by thinking of density-functional methods in terms of effective Kohn–Sham potentials, one could arrive at new physical insights and better approximations for computing molecular properties. **Nikitas Gidopoulos (**Rutherford Appleton Laboratory, U.K.) concentrated on progress at the interface of wave function and density functional theories. He presented recent work that gave a fresh viewpoint to some basic questions in DFT, for example, why it is physically meaningful to consider the effective Kohn Sham (KS) system in place of the interacting system.

The next two sessions were devoted to functionals and potentials in DFT. Andreas Savin concentrated on choosing the best density functional approximation, illustrating his point with results obtained for band gaps of solids. He showed that different criteria can lead to different choices for the “best functional”. To decide which specific density functional approximation should be used can thus be made only by introducing some supplementary, external, possibly personal criterion. **Wei Ku** (Brookhaven National Laboratory) presented first-principles, Wannier-function based methods for disordered

materials and their applications. His Wannier function based method is systematically improvable, beyond-mean-field, and not perturbation limited. Case studies were discussed include dilute magnetic semiconductors, transition metal oxides, and Fe-based superconductors. **Thomas Hollins** (University of Durham) discussed optimized effective potentials using the Hylleraas variational method. In electronic structure calculations the optimized effective potential (OEP) is a method that treats exchange interactions exactly using a local potential within DFT. The method has been implemented within the plane-wave, pseudopotential formalism. Electronic structures for group IV, III-V and II-V semiconductors as well as group I-VII insulators have been calculated using the OEP and compared to calculations using the local density approximation (LDA), a selection of generalized gradient approximations (GGAs) and Hartree-Fock (HF) functionals. **Valentina Brosco** (Universià di Roma) presented a work on Exact Exchange-correlation Potential of a correlated insulator with a free surface. In particular, it was shown that the discontinuity of the effective potential has a sizable effect on the gap even in the weakly correlated regime and, as expected, it became dominating in Mott regime. In addition a new correlation induced barrier was shown to form in the effective potential on the surface between bulk and vacuum. **Weitao Yang** (Duke University) concentrated on fractional perspectives of density functional theory. The theory is widely and successfully applied in simulations throughout engineering and sciences. However, there are major failures for many predicted properties. These errors can be characterized and understood through the perspective of fractional charges and fractional spins introduced recently. The fractional perspectives offer a possible pathway forward. He reported progress in excited states, spin state splitting, open- shell singlet states, fukui functions and band gaps. **Nektarios Lathiotakis** (National Hellenic Research Foundation) explained his work on constraining the Optimized Effective Potential to correct self-interactions, as well as applications to density and reduced-density-matrix functionals. Self-interaction is a major problem in density functional approximations and the source of serious divergence from experimental results. He proposed to minimize any density functional with respect to an effective optimized potential under additional constraints that guarantee that this potential is asymptotically correct. Thus, it should be possible to correct SIs from the potential rather than the functional. **C. Z. Wang** (Iowa State University) gave an overview of a development of first-principles methods for strongly correlated electrons in solids and molecules. **J. Lorenzana** (University of Rome) discussed Density Functional Theory with adaptive pair density. He proposed a density functional to find the ground state energy and density of interacting particles, where both the density and the pair density can adjust in the presence of an inhomogeneous potential. As a proof of principle he formulated an a priori exact functional for the inhomogeneous Hubbard model. The functional had the same form as the Gutzwiller approximation but with an unknown kinetic energy reduction factor which encodes all the complication of the many-body problem.

The next session was devoted to issues relevant for practical applications of the theory in materials modeling, and concentrated on temperature effects in simulations of alloys and compounds. The combination of accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts has quickly advanced in the past few years and allows now to tackle even the complexity of advanced engineering materials. Key to these studies is the highly accurate determination of free energies. **Jörg**

Neugebauer (Max-Planck-Institut für Eisenforschung, Düsseldorf) explained new techniques for fully *ab initio* determination of materials properties at finite temperatures. He showed how efficient sampling strategies together with highly converged density-functional theory calculations allow an unbiased and accurate determination of all relevant temperature dependent free energy contributions. The flexibility and the predictive power of this approach was discussed for examples relevant to the design and understanding of modern high strength steels or light weight metallic alloys. **Patrice Turchi** (Lawrence Livermore National Laboratory) discussed electronic structure and thermodynamics of actinide-based alloys. Although the impact of electron correlations on actinide alloy properties is still under assessment, he showed how current state-of-the-art *ab initio* methods can shed light on phase stability and tendencies towards order or phase separation in mixtures of actinide elements (U, Np, Pu, Am), either among themselves or with transition metals such as Mo and Zr. **Daniel Grieger** (Universität Hamburg) presented a case study finite-temperature phase diagrams of strongly correlated material V_2O_3. A key step was to converge the correlated charge density within a comprehensive LDA+DMFT interface (charge self-consistency). **Vsevolod Razumovskiy** (KTH, Sweden) illuminated vacancy cluster mechanism of metal atom diffusion in sub-stoichiometric carbides. The energetics of the metal and carbon atom self-diffusion in TiC and ZrC carbides was studied by means of first principles calculations. A new type of stable point defect cluster was predicted to form in sub-stoichiometric TiC and ZrC carbides – a metal vacancy ”dressed” in a shell of up to six carbon vacancies. **Alberto Marmodoro** (University of Warwick and Max-Planck-Institut für Mikrostrukturphysik Weinberg) continued his efforts for the first principles study of disordered systems, in order to generalize the non-local CPA / DCA to the case of complex unit cell materials with more than one sublattice. He presented a multi-sublattice extension of the non-local CPA for complex disordered materials.

Following sessions were dedicated to many-body methods. **Pina Romaniello** (Université Paul Sabatier, Toulouse) suggested a technique that goes beyond the GW approximation. Correlation in the framework of Many-Body Perturbation Theory (MBPT) was discussed, starting from the GW approximation and going beyond. GW properly describes the high-density regime, where screening was important; in the low-density regime, instead, other approximations were proposed. **J. A. Berger (**European Theoretical Spectroscopy Facility) presented the effective-energy technique to evaluate in an accurate and numerically efficient manner electronic excitations by reformulating spectral sum-over-states expressions such that only occupied states appear. In **Qingguo Feng** (Linköping University) work the equations of motion were extensively studied. Several impurity solvers are successful constructed for both single orbital and multi-orbital systems in different physical situations by calculating the equations of motion and then making these equations closed with a truncation/decoupling scheme. **S. Karoui** (ONERA-CNRS) investigated order and size effects in late transition metals through many body methods, and affirmed that magnetism and chemical order are unequivocally interrelated, and quantifiable with an enthalpy gain. **Viraht Sahni** (Brooklyn College) presented a survey on recent developments in Density Functional Theory in the presence of a magnetostatic field. He argued [5] that definitions of density functional theory arrived at via proofs of bijectivity between basic variables and external potentials, as in the original Hohenberg-Kohn theorem and our present work, are more fundamental than

the constrained-search definitions of Percus-Levy-Lieb. **M. Däne (**Lawrence Livermore National Laboratory) described self-interaction free and analytic treatment of the coulomb energy in Kohn-Sham DFT. The pair density was expressed explicitly in terms of the density using a orthonormal and complete basis expressed as a functional of the density. The method was illustrated with numerical results for the atom series. Tony Gonis (Lawrence Livermore National Laboratory) showed that the theorems of Hohenberg and Kohn can be derived strictly through the constrained search without the *a priori* assumption of *v*-representability. Based on the explicit calculation of functional derivatives with respect to the density, the formalism of Kohn and Sham is expressed in a form that avoids by construction the problem of self-interaction in the treatment of the Coulomb energy. **Vladimir Antropov** (Ames Laboratory) presented his consistent theory of magnetism and superconductivity in iron superconductors. **Joseph Betouras** (Loughborough University) concentrated on paradigms of Lifshitz Topological Transitions in systems of interacting fermions, involving (i) dipolar fermions in optical lattices and (ii) itinerant electrons close to a ferromagnetic quantum critical point but in the disordered side. **M. Yu. Lavrentiev** (EURATOM/CCFE) showed how the complex interplay between magnetic properties, short-range order, and effects of phase decomposition of iron-chromium alloys can be described using Magnetic Cluster Expansion.

Part of the workshop devoted to correlations in alloys was opened by **B. Alling** (linköping University), who presented a new technique for first-principles treatment of paramagnetism by Disordered Local Moments Molecular Dynamics (DLM-MD) with application to CrN and (Cr-Al)N alloys. In the work of **L. V. Pourovskii** (CPHT-Ecole Polytechnique) state-of-the-art fully self-consistent and full-potential *ab initio* simulations within the dynamical mean-field theory were employed to study properties of iron at extreme conditions, resulting in a prediction that all three possible structures of Fe should have sufficiently high magnetic susceptibility to stabilize the geodynamo. **Igor Di Marco** (Uppsala University) discussed LDA+DMFT implementation based on a Full-Potential Linear Muffin-Tin Orbital method (FP-LMTO) and the application of the technique in studies of local correlation effects in the electronic structure of Mn doped GaAs. **Leon Petit** (Daresbury Laboratory) used the self-interaction corrected (SIC) local spin density approximation to describe the dual, localized-delocalized, character of 5*f*-electrons in actinide metals and compounds. **I. Leonov** (University of Augsburg) present results of a theoretical investigation of the electronic and lattice dynamical properties of elemental iron at finite temperatures obtained within dynamical mean-field theory implemented with the frozen-phonon method. In large scale dynamical cluster quantum Monte Carlo simulations of the two-dimensional (2D) Hubbard model with only nearest neighbor hopping, **M. Jarrell** (Louisiana State University) found a quantum critical point at finite doping separating a Fermi liquid region at low filling from a non-Fermi liquid pseudogap region near half-filling. Very interesting works on magnetism and superconductivity were presented by **M. W. Long** (Birmingham University), **Hai-Ping Cheng** (University of Florida) **Balazs Ujfalussy** (Wigner Research Centre for Physics), while more applied aspects of the theory were discussed by **A. Landa** (Lawrence Livermore) and **Igor Abrikosov** (Linköpping University). The last day of the conference was devoted to properties of alloys and compounds, as well as to advances in time-dependent methods.

Assessment of the results and impact of the event on the future direction of the field (up to 2 pages)

The science of electron correlations is of crucial interest in wide classes of materials consisting of pure elemental solids, such as transition, rare earth and actinide metals as well as compounds such as metal oxides, where standard Density Functional Theory (DFT) based approaches, such as the Local Density Approximation (LDA), Generalized Gradient Approximation (GGA), may not provide a robust description of even the ground state electronic and structural properties, much less those of excited states and reaction pathways. Clearly, the development of coherent, parameter free and efficient electronic structure methodologies for such materials could have a direct impact in areas ranging from understanding the mechanism responsible for high temperature superconductivity to the development of the next generation of nuclear reactors.

It is also generally recognized that electron correlations play a singular role in alloys of transition metals in determining such physical properties as magnetism, while also being responsible for the behavior of semiconductors as well as wide gap insulators. Indeed, in recent developments, such methodologies as the LDA+U and the dynamical mean field theory (DMFT) are being applied in attempts to understand and predict the properties of alloys and compounds. In this regard, the first-principles calculation of alloy phase diagrams, the road maps of alloy engineering, remain a crucial point of concern. Being able to extend methodologies for studying the effects of the Coulomb interaction to alloys is a particularly needed development.

While no general approach or grand synthesis has yet emerged for dealing with the subtleties of correlated electron behavior, a wide variety of methods have been, and continue to be, developed that capture important aspects of the problem. Amongst these can be counted methodologies directly related to DFT, such as optimized effective potential methods (OEP), hybrid functional approaches, LDA+U, the Dynamical Mean Field Theory (DMFT) and Dynamical Cluster Approximation (DCA), the GW approximation and its self-consistent extension, the recent advances based on the Gutzwiller wave function, the two-particle treatment of correlations, and the relation of these methodologies to long established Density Functional Theory (DFT).

Indeed, methodologies developed in connection with one field find immediate application in the other, such as, for example, the DCA. Initially developed with respect to correlated systems it is applicable to alloys where it provides an extension of the single-site coherent approximation (CPA) to a cluster theory. Clearly, the formal and computational bounds between alloy physics, materials science and first-principle methodology for the treatment of correlation are being blurred. At the same time, the application of the methods just mentioned to disordered materials is at its infancy, if that! The time is ripe for a concerted effort to mesh formal advances in the study of correlations with the special formalisms developed for the study of the electronic structure of disordered alloys.

Through exposure and communication of both theoretical developments and their applications to real systems and comparison to experiment, the **International Symposium and Workshop on Electron Correlations and Materials properties of**

Alloys and Compounds identified methodologies that address the effects of correlations on the properties of materials, and provided a comparative understanding of the advantages and limitations of each method thus motivating further research. Deep, person-to-person discussions of fundamental elements in the study of correlated electrons in matter, including elemental solids, compounds and alloys helped sustain existing research, enhance and motivate new developments and also should promote new as well as presently active collaborations between Laboratory scientists and their colleagues elsewhere. Such personal interactions had an energizing and beneficial effect in further developments of the field. During the **General Discussion** session led by *Malcolm STOCKS* participants fully agreed that the meeting was highly successful and suggested to establish a new conference series, where two research communities continue to meet. It was also suggested that future conferences should contain introductory overview talks on respective fields, strong electron correlations and simulations of properties of alloys and compounds, aimed at summarizing recent developments and challenges of the fields. This should give good introduction for both communities into the current status of the respective fields, and promote further cross-disciplinary communications during the conferences. These keynote presentations should be given by leading experts in theory of strong electron correlations and the alloy theory.

Final programme of the meeting

Sunday, July 8th

17:00-19:00	**REGISTRATION**
19:00	**DINNER**

Monday Morning (Mm), July 9th

08:15		*WELCOME - Organizers of ECMPCA*
		Wave-Function-based DFT **Chair:** *Viktor STAROVEROV*
08:30	Mm1	***Rodney BARTLETT,*** Matthew Strasberg, Ajith Perera, and Prakash Verma Some ruminations on correlated orbital theories and the existence of a consistent density functional theory
9:00	Mm2	***Andreas THEOPHILOU*** and Iris Theophilou On the quality of the Kohn and Sham wave functions
9:30	Mm3	***Viktor STAROVEROV*** Advances in methodology and applications of model Kohn–Sham potentials
10:00	Mm4	***Nikitas GIDOPOULOS*** Progress at the interface of wave-function and density functional theories
10:30		**COFFEE BREAK**

		Functionals and Potentials in DFT: I **Chair:** *Nektarios LATHIOTAKIS*
11:00	Mm5	***Andreas SAVIN,*** Bartolomeo Civalleri, Davide Presti, and Roberto Dovesi On choosing the best density functional approximation
11:30	Mm6	***Wei KU*** First-principles Wannier function based methods for disordered materials and applications to studies of oxides and Fe-superconductors
12:00	Mm7	***Thomas HOLLINS,*** S.J. Clark, and N. I. Gidopoulos Optimized effective potential using the Hylleraas variational method
12:30	Mm8	***Valentina BROSCO,*** Zujian Ying, and Josè Lorenzana Exact exchange-correlation potential of a correlated insulator with a free surface
13:00-15:00	**WELCOME RECEPTION**	

Nota Bene: Each presentation is referred to by the day (**M**=Monday, **Tu**=Tuesday, **W**=Wednesday, **Th**=Thursday, **F**=Friday), followed by **m** (morning), **a** (afternoon), or **e** (evening), and the order of occurrence in the session. For the evening session on Tuesday, the number locates the board on which the presentation will be posted.

Monday Afternoon (Ma), July 9th

		Functionals and Potentials in DFT: II **Chair:** *Rodney BARTLETT*
17:00	Ma1	***Weitao YANG,*** Aron J. Cohen, Paula Mori-Sanchez, E.R. Davidson, Xiangqian Hu, Xiao Zheng, Daniel Ess, Frank DeProft, and Paul Geerlings Fractional perspectives of density functional theory
17:30	Ma2	***Nektarios LATHIOTAKIS,*** N. I. Gidopoulos, and N. Helbig Constraining optimized effective potential to correct self-interactions: Applications to density and reduced-density-matrix functionals
18:00	Ma3	***Cai-Zhuang WANG*** Development of first-principles methods for strongly correlated electrons in solids and molecules
18:30	Ma4	***Jose LORENZANA,*** Z.-J. Ying, and V. Brosco Density functional theory with adaptive pair density
19:00	**DINNER**	

Tuesday Morning (Tum), July 10th

Alloys and Compounds - Temperature Effects **Chair:** *Peter HIRSCHFELD*		
08:30	Tum1	***Jörg NEUGEBAUER,*** Fritz Körmann, Blazej Grabowski, and Tilmann Hickel Fully *ab initio* determination of materials properties at finite temperatures
09:00	Tum2	***Patrice TURCHI,*** A. I. Landa, V. Lordi, and Per Söderlind Electronic structure and thermodynamics of Actinide-based alloys
09:30	Tum3	***Daniel GRIEGER,*** Christoph Piefke, Oleg E. Peil, and Frank Lechermann Approaching finite-temperature phase diagrams of strongly correlated materials: A case study for V_2O_3
10:00	Tum4	***Vsevolod RAZUMOVSKIY,*** A. V. Ruban, J. Odqvist, and P. A. Korzhavyi Vacancy cluster mechanism of metal atom diffusion in sub-stoichiometric carbides
10:30	Tum5	***Alberto MARMADORO,*** Arthur Ernst, and Julie B. Staunton Multi-sublattice extension of the non-local CPA for complex disordered materials
11:00	**COFFEE BREAK**	
Many -Body Methods: I **Chair:** *Mark JARRELL*		
11:30	Tum6	***Antoine GEORGES*** Strong correlations from Hund's rule coupling
12:00	Tum7	***Pina ROMANIELLO*** Beyond the GW approximation: combining correlation channels
12:30	Tum8	***Arjan BERGER,*** L. Reining, and F. Sottile Efficient GW calculations for SnO_2, ZnO and rubrene: the effective energy technique
13:00	**LUNCH**	

Tuesday Afternoon and Evening (Tua–Tue), July 10th

Many -Body Methods: II **Chair:** *Balazs UJFALUSSY*		
17:00	Tua1	***Qingguo FENG*** Fast impurity-solvers for dynamical mean-field theory based on equation of motion approach
17:30	Tua2	***Sonders KAROUI,*** H. Amara, and F. Ducastelle Order and size effects in late transition metals reflected through many-body methods
18:00-19:30	**Evening Session: Tue1 – Tue11**	
19:30	**DINNER**	

Wednesday (Wm), July 11th

Formal Developments in DFT **Chair:** *Aristides MAVRIDIS*		
08:30	Wm1	***Mel LEVY*** New variational principles in density-functional theory for ground states and excited states and for degeneracies and non-degeneracies
09:00	Wm2	***Viraht SAHNI*** and Xiao-Yin Pan Recent developments in density functional theory in the presence of a magnetostatic field
9:30	Wm3	***Markus DÄNE,*** Antonios Gonis, D. M. Nicholson, and G. Malcom Stocks Self-interaction free and analytic treatment of the Coulomb energy in Kohn-Sham Density Functional Theory
10:00	Wm4	***Antonios GONIS,*** Markus Däne, D. M. Nicholson, and G. M. Stocks Density functional theory without Hohenberg and Kohn and self-interaction free Coulomb and correlation energy in the Kohn-Sham formulation
10:30	**COFFEE BREAK**	
Magnetism and Superconductivity: I **Chair:** *Wei KU*		
11:00	Wm5	***Vladimir ANTROPOV,*** Mark van Schilfgaarde, and Mikhail I. Katsnelson Consistent theory of magnetism and superconductivity in iron superconductors
11:30	Wm6	***Joseph BETOURAS,*** Sergey Slizovskiy, Sam Carr, and Jorge Quintanilla Paradigms of Lifshitz topological transitions in systems of interacting fermions
12:00	Wm7	***Peter HIRSCHFELD*** Defects in strongly correlated metals and superconductors
12:30	Wm8	***Mikhail LAVRENTIEV,*** D. Nguyen-Manh, and S. L. Dudarev Magnetic cluster expansion model for magnetic properties of Fe-Cr alloys
13:00	**WEDNESDAY AFTERNOON: excursion**	
19:00-22:00	**Greek Night: CONFERENCE DINNER**	

Thursday Morning (Thm), July 12th

Alloys and Compounds - Correlations **Chair:** *Hai-Ping CHENG*		
08:30	Thm1	***Bjorn ALLING,*** P. Steneteg, T. Marten, and I. A. Abrikosov First-principles treatment of paramagnetism by disordered local moments-molecular dynamics (DLM-MD): the example of CrN
09:00	Thm2	***Leonid POUROVSKII*** Electronic correlations in iron metal at extreme conditions
09:30	Thm3	***Igor di MARCO,*** Patrik Thunström, and Olle Eriksson Local correlation effects in the electronic structure of Mn doped GaAs
10:00	Thm4	***Leon PETIT,*** Zdzislawa Szotek, Walter Temmerman, and Martin Lüders

		SIC-LSD calculations of Actinide metals and alloys
10:30	Thm5	***Ivan LEONOV*** Electron correlations and lattice dynamics of elemental iron near the α–γ phase transition
11:00	**COFFEE BREAK**	
Magnetism and Superconductivity: II **Chair:** *Andreas THEOPHILOU*		
11:30	Thm6	***Mark JARRELL,*** J. Moreno, S. Yang, K. Chen, and Z. Meng Quantum criticality and Superconductivity in the Hubbard model
12:00	Thm7	***Martin LONG*** and A. K. A Briffa The long-range dipole interaction in anti-ferromagnetic pyrochlores: The exotic magnetism of $Gd_2Ti_2O_7$
12:30	Thm8	***Hai-Ping CHENG,*** Yu-Ning Wu, and Xiao-Guang Zhang Molecular magneto-capacity
13:00	Thm9	***Balazs UJFALUSSY*** and Eszter Simon Magnetic interactions on alloy surfaces
13:30	**LUNCH**	

Thursday Afternoon (Tha), July 12th

Alloys and Compounds - Stability **Chair:** *Vladimir ANTROPOV*		
17:00	Tha1	***Alexander LANDA,*** P. Söderlind, O. I. Velikokhatnyi, I. I. Naumov, A. V. Ruban, L. Vitos, and O. E. Peil Alloying-driven phase stability in group-VB transition metals under compression
17:30	Tha2	***Igor ABRIKOSOV*** Correlated electrons in technological materials
18:00- 19:30	**General Diuscussion** **Chair: *Malcolm STOCKS***	
19:30	**DINNER**	

Friday Morning (Fm), July 13th

Alloys and Compounds - Properties **Chair:** *Martin LONG*		
08:30	Fm1	***Perla WAHNON,*** P. Palacios, Y. Seminovski, J. C. Conesa, and R. Lucena Obtaining novel In-gap electronic structures through metal inclusion in In and Sn sulphides: Quantum modeling and experimental realizations
09:00	Fm2	***Stephan SCHÖNECKER,*** B. Johansson, and L. Vitos Surfaces parameters of ferritic stainless steels

09:30	Fm3	***Aristides MAVRIDIS*** and Apostolos Kalemos Structure and Bonding of Sc_2, Ti_2, and Mn_2
10:00	Fm4	***Xiaoqing LI,*** Hualei Zhang, Song Lu, Wei Li, Jijun Zhao, Börje Johansson, and Levente Vitos Elastic properties of V-based alloys from first-principles theory
10:30	**COFFEE BREAK**	
	Time-Dependent Methods **Chair:** *Svetlana BARANIKOVA*	
11:00	Fm6	***Stefan KURTH*** The derivative discontinuity in transport: towards a density functional description of Coulomb blockade and Kondo effect
11:30	Fm7	***Claudio VERDOZZI*** TDDFT dynamics for strongly correlated lattice systems
12:00	***CLOSING REMARKS - Organizers of ECMPCA***	
12:30	**LUNCH**	

EVENING SESSION

Tuesday, July 10th (Tue), 18:00–19:30

Tue1. ***Petros SOUVATZIS***
Phonon lifetimes from first-principles self-consistent lattice dynamics

Tue2. ***Svetlana BARANNIKOVA,*** A. V. Ponomareva, L. B. Zuev, Yu. Kh. Vekilov, and I. A. Abrikosov
Significant correlation between macroscopic and microscopic parameters for the description of localized plastic flow auto-waves in deforming Fe-based alloys

Tue3. ***Ivan BLESCOVT,*** T. Hickel, and J. Neugebauer
Ab initio investigation of stacking faults in Fe-based alloys

Tue4. ***Nektarios LATHIOTAKIS*** and Z. G. Fthenakis
A theoretical study of graphene and its planar allotropes under extreme uniaxial strain

Tue5. ***Oscar GRÅNÄS,*** Igor di Marco, Olle Eriksson, Lars Nordström, and Corina Etz
Assessment of the magnetic properties and electronic structure of $SrRuO_3$ using LDA, LDA+U, and LDA+DMFT

Tue6. ***Maria TASSI,*** Iris Theophilou, Peter Grünberg, and S. Thanos
Ab initio calculations for doubly excited states

Tue7. ***Sam FAULKNER***
Recent developments in multiple scattering theory

Tue8. ***Hunter SIMS,*** W. H. Butler, M. Richter, and K. Koepernik
Theoretical investigation into the possibility of very large moments in $Fe_{16}N_2$

Tue9. ***Luiz Claudio de CARVALHO,*** A. Schleife, J. Furthmüller, and F. Bechstedt
Excitonic and quasiparticle effects on optical properties of $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ alloys: A first principles study

Tue10. ***Mikhail PETRIK*** and Y.N.Gornostyrev
The effect of magnetism on the solubility and interaction energy of solute atoms in IrN-based alloys

Tue11. ***Antonios GONIS,*** Markus Däne, and D. M. Nicholson
On the N-representability of the pair density