16th International Conference on Density Functional Theory and its Applications

Conference Programme

The venue of the conference is Kölcsey Központ (Kölcsey Convention Center)

(4026 Debrecen, Hunyadi u. 1-3.) It is in the center of Debrecen.

http://www.vistahungary.com/index.php?lang=en&id=624&menu_id=589

All the lectures, posters, coffees, lunches, the registration and the get-together party on Monday will be there.

The reception on Thuesday will be in the Main Building of the University of Debrecen (4032, Egyetem tér 1.). The Banquet will be in the Erdőspuszta - Fenyves Vendéglő Restaurant (4002 Debrecen, Diószegi - Panoráma út crossroads).

Monday, August 31, 2015

17.00 - 19.00 Registration

19.00 - 22.00 Get-together party

Tuesday, September 1, 2015

Chair: Ágnes Nagy

8.45 - 9.00	Opening
9.00 - 9.40	**Mel Levy,** Duke, USA
	Perspectives on Variational Principles in Time-Independent Density-Functional Theory and
keynote	Total Energy as a Simple Sum of Shifted Kohn-Sham Orbital Energies
9.40 - 10.10	**Fabio Della Sala,** Lecce, Italy,
invited	Kinetic energy density in the nuclear and asymptotic regions
10.10 - 10.40	**Coffee**

Chair: Andreas Theophilou

10.40 - 11.10	**Vitaly Glushkov,** Dnipropetrovsk,Ukrain,
invited	Orthogonality constrained local potential method for doubly excited states
11.10 - 11.40	**Katarzyna Pernal,** Lodz, Poland,
invited	Excitation energies from based on ensemble variational principle
11.40 - 12.00	**Prasanjit Samal,.**Bhubaneswar, India
	Uniqueness, Existence, and Construction of the Density-to-Potential Mapping for Excited-States
12.00 - 13.00	**Lunch**

Chair: Karlheinz Schwarz

13.30 - 14.00	**Gábor Csonka**, Budapest, Hungary,
invited	Random Phase Approximation: new developments and applications
14.00 - 14.30	**Börje Johansson**, Stockholm, Sweden,
invited	Structural properties of the lanthanides and actinides from DFT
14.30 - 15.00	**Hubert Ebert**,.Munich, Germany,
invited	Response functions in Spintronics calculated by means of the Kubo formalism
15.00 - 15.30	**Jean-Philip Piquemal,** Paris, France,
invited	Unraveling non-covalent interactions within flexible biomolecules: coupling electron density topology to first principle molecular dynamics and DFT/MM
15.30 - 16.00	**Coffee**

Chair: Kieron Burke

16.00 - 16.40	**John Perdew**, Temple, USA
	(Like 50 Million Frenchmen) Can't Be Wrong?
keynote	SCAN Meta-GGA: Seventeen Exact Constraints
16.40 - 18.40	**Posters A**
19.30 -22.00.	Reception (Main Building of the University, Egyetem tér 1)

Wednesday, September 2, 2015

Chair: Eberhard Gross

9.00 - 9.40 *keynote*	**Kieron Burke**, California, USA, Removing most self-interaction errors from density functional calculations
9.40 - 10.10 *invited*	**Rex Godby**, York, UK, Exact correlation and localisation in model time-dependent systems
10.10 - 10.40	**Coffee**

Chair: Dennis R. Salahub

10.40 - 11.10 *invited*	**Mark Casida**, Grenoble, France, The Challenge of Photochemistry for Time-Dependent Density-Functional Theory
11.10 – 11.40 *invited*	**Nicole Helbig**, Jülich, Germany, Rabi oscillations in time-dependent density functional theory
11.40 – 12.00	**Denis Jacquemin**, Nantes, France On the relative performances of TD-DFT and GW /BSE for describing the excited-states of molecular systems
12.00 - 13.00	**Lunch**
13.30 - 15.00	**Short oral presentations A, B, C**
15.30 - 17.30	**Sight-seeing**
19.00 - 22.00	**Banquet** Erdőspuszta - Fenyves Vendéglő Restaurant (4002 Debrecen, Diószegi - Panoráma út crossroads)

Short oral presentations A

Chair: Claudio Amovilli

13.30 - 13.40	**Jan Gerit Brandenbur**, Bonn, Germany Consistent structures and interactions by density functional theory with small basis sets
13.40 – 13.50	**Du Zhang**, Durham, USA Excitation energies, analytic gradients and potential energy surfaces from the particle-particle random phase approximation
13.50 – 14.00	**Jilai Li**, Berlin, Germany Distinct Mechanistic Differences in the Hydrogen-Atom Transfer from Methane and Water by the Heteronuclear Oxide Cluster
14.00 - 14.10	**Aurélien Moncomble**, Lille, France Solvent effects to compute UV-vis spectra for ionic metal complexes
14.10 – 14.20	**Mátyás Pápai**, Budapest, Hungary Theoretical Investigation of the Light-Induced Spin Transition in the [Fe(terpy)2]2+ Complex
14.20 - 14.30	**Emese Rozsalyi**, Budapest, Hungary Theoretical Study of Light-Induced Processes in Fe(II) Complexes
14.30 - 14.40	**Dumitru-Claudiu Sergentu**, Nantes, France Electronic structures of the XF3 (X = Cl, Br, I, At) fluorides and topology of their potential energy surfaces
14.40 - 14.50	**Marietjie Ungerer**, Potchefstroom, South Africa Molecular Modelling of Tantalum Penta-Halides A comparative DFT study
14.50 – 15.00	**Kazuyoshi Ogasawara Sanda**, Japan First-Principles Calculation of Color of Ruby

Short oral presentations B

Chair: Kalevi Kokko

13.30 - 13.40	**Dongyoo Kim**, Stockholm, Sweden Magnetic Properties of L10-MnGa/Co(001) Films Depending on Interface Structure and Epitaxial Strain
13.40 - 13.50	**Shaoqing** Wang, Shenyang, China Vibrational spectrum analysis on the rippled structure of graphene
13.50 - 14.00	**Andreas Erlebach**, Jena, Germany Structure Evolution of Nanoparticulate Fe2O3: Synergy Between Theory and Experiment
14.00 - 14.10	**Lukas Gajciar,** Jena, Germany Low-memory iterative density fitting: towards routine DFT calculations on molecules with thousands of atoms
14.10 - 14.20	**Dmytro Kandaskalov**, Marseille, France Microstructural evolution of martensite at low temperature
14.20 - 14.30	**Mauricio Antonio Rodriguez-Mayorga**, Girona, Spain On the effect of electron correlation in 3-RDM proximations.
14.30 - 14.40	**Roberto Rivelino,** Bahia, Brazil Tuning the Metal-Semiconductor Transition in 2D Metallic Silicon-Boron Materials by Hydrogenation
14.40 - 14.50	**Balázs Újfalussy**, Budapest, Hungary Critical temperature of superconductor-normal metal heterostructures

Short oral presentations C

Chair: Paul Geerlings

13.30 - 13.40	**Eloy Ramos-Cordoba,**Donostia, Spain Understanding and quantifying electron correlation
13.40 - 13.50	**Marco Franco-Pérez**, Iztapalapa, México The electronic charge transference phenomena in DFT at finite temperatures
13.50 - 14.00	**Ferenc Tasnádi**, Linkoping, Sweden Advanced properties of alloys - First-principles studies of TiAlN alloys and TiAlN/TiN(001) multilayers
14.00 - 14.10	**Kaito Miyamots**, Bristol, UK Embedded Mean-Field Theory
14.10 - 14.20	**Eduardo Fabiano**, Lecce, Italy Study and application of a new gradient-dependent upper bound of the exchange-correlation energy
14.20 - 14.30	**Jorge Garza**, Iztapalapa, Mexico Performance of exchange-correlation functionals on confined many-electron atoms
14.30 - 14.40	**László von Szentpály**, Stuttgart, Germany Thermocyclic Equations and Symmetry Laws to Explain and Limit Conceptual DFT Principles
14.40 - 14.50	**Emmanuel Fromager**, Strasbourg, France Linear interpolation method in ensemble Kohn-Sham and range-separated density-functional proximations for excited states
14.50 - 15.00	**Andreas Ostlin**, Stockholm, Sweden The virial theorem within many-body extensions of density functional theory
15.30 - 17.30	**Sight-seeing**
19.00 - 22.00	**Banquet** Erdőspuszta - Fenyves Vendéglő Restaurant (4002

Debrecen, Diószegi - Panoráma út crossroads)

Thursday, September 3, 2015

Chair: David J. Tozer

9.00 - 9.40	**Ann Mattsson**, Sandia,USA
keynote	Towards a Density Functional Theory exchange-correlation .functional for d- and f-electron elements and compounds
9.40 - 10.10	**Paola Gori-Giorgi**, Amsterdam, Netherland
invited	Functionals from the strong-coupling limit of DFT: promises and challenges
10.10 - 10.40	**Coffee**

Chair: Henry Chermette

10.40 - 11.10	**Luuk Visscher**, Amsterdam, Netherland,
invited	Combining electronic structure methods with subsystem DFT Theory and Applications
11.10 - 11.35	**Presentation in memory of Tom Ziegler**
	Evert Jan Baerends
11.35 - 12.00	**Mykhaylo Krykunov**, Calgary, Canada
	Electronic excitations in transition metal complexes through the prism of constricted variational density functional theory
12.00 - 13.10	**Lunch**
13.10 - 13.40	Sponsor Presentation by SCM
	Stan van Gisbergen

New DFT(B) methods and applications in the ADF suite

Chair: Claude A. Daul

13.40 - 14.10	**Olle Eriksson**, Uppsala, Sweden
invited	Electronic structure theory of nano-sized objects from LDA to DMFT
14.10 - 14.30	**Josep M Luis**, Girona, Spain
	Design and characterization of molecular electrides
14.30 - 14.50	**Li Chen**, Durham, USA
	Local Scaling Correction for Reducing Delocalization Error in Density Functional Approximations
14.50 - 15.10	**János Ángyán**, Vandoeuvre-les-Nancy, France
	Van der Waals Corrected DFT Methods and their Application to Adsorption of Volatile Organic Compunds in Zeolites
15.10 - 15.30	**Martin Dracinsky**, Prague, Czech Republic
	Nuclear delocalization of hydrogen atoms studied by PIMD simulations and NMR spectroscopy
15.30 - 16.00	**Coffee**

Chair: Jose M. Garcia de la Vega

16.00 - 16.20	**Nikitas Gidopoulos**, Durham, UK
	Taylor-series expansions of the Kohn-Sham potential
16.20 - 16.40	**Elvira Romera**, Granada, Spain
	Density Functional Fidelity Susceptibility, Relative Rényi Entropies and Quantum Phase Transitions
16.40 - 17.00	**Vincent Tognetti**,.Normandy Univ., France
	New conceptual DFT descriptors for reactivity
17.00 - 17.20	**Marcel Swart**, Barcelona, Spain
	Exchange interactions in transition-metal reactivity
17.20 - 17.40	**Bartolomeo Civalleri**, Torino, Italy
	Double-hybrid density-functional theory applied to

	solids
17.20 - 19.20	**Posters B**

Friday, September 4, 2015

Chair: Evert Jan Baerends

9.00 - 9.40	**Andreas Savin**, Sorbonne, France
keynote	Pitfalls of statistics used in judging the performance of theoretical models in quantum chemistry
9.40 - 10.10	**Chandre Dharma-wardana**, Ottawa, Canada
invited	Current issues in finite-Temperature density functional and warm correlated matter
10.10 - 10.40	**Coffee**

Chair: Agnes Nagy

10.40 - 11.10	**Paul Ayers**, McMaster, Canada
invited	Time-Independent Theories for Multiple Excited States
11.10 – 11.30	**Eduard Matito, Donostia** International Physics Center, Spain
	Harmonium atom as a calibration and development tool in DFT
11.30 - 11.50	**Jeng-Da Chai**,.Taipei, Taiwan
	TAO-DFT and Its Applications to Zigzag Graphene Nanoribbons

11.50 - 12.00	**Closing**
12.00 - 13.30	**Lunch**