PROGRAM – DFG1178 ANNUAL REPORT COLLOQUIUM AND ECDM5 (GRAVEDONA 6–11 June 2008)

Friday, June 6	
	Arrival in Gravedona (transportation from Milano airports available in the late afternoon (Departure from Milano Malpensa or Milano Linate approx. at 18.00)
	Registration
21:00-23:00	**DFG Welcome Party at Palazzo Gallio, Gravedona**

Saturday, June 7		
08:30 – 08:45		**Opening Cerimony**
08:45 – 09:00	Stalke/ Jansen	**Introductory Remarks**
09:00 – 09:50	**D. Stalke**	**KN 2: What Can a Synthetic Chemist Learn From Charge Density?**
09:50 – 10:10	U. Flierler	$[(thf)Li_2\{H_2CS(N^tBu)_2\}]_2$: Synthesis, Polymorphism, and Experimental Charge Density to Elucidate the Bonding Properties of a Lithium Sulfur Ylide
10:10 – 10:30	V. H. Gessner	Experimental Charge Density Studies of Organolithium Compounds
10:30 – 10:35	*Time for Discussion*	
10:35 – 11:00	**Coffee Break**	
11:00 – 11:20	N. W. Mitzel	On the Nature of Intramolcular Dative Bonds in Silanes with Donor Functions in Close Proximity
11:20 – 11:40	H. Braunschweig	Electron Density Investigation of the Dinuclear Borylene Complex $[\{Cp(CO)_2Mn\}_2(\mu\text{-}B^tBu)]$
11:40 – 11:45	*Time for Discussion*	
11:45 – 12:05	D. Lentz	Experimental Charge Density Determination of closo-Hydroborates
12:05– 12:25	U. Englert	Electron Density Study on One-Dimensional Coordination Polymers
12:25 – 12:30	*Time for Discussion*	
12:30 – 14:30	**Lunch**	
14:30 – 15:20	**S. Dahaoui**	**KN 8: Understanding the Halogen...X (X=Halogen, Lewis Base) interactions: Application to charge transfer complexes**
15:20 – 15:40	W. Scherer	On the Electronic Structure of the Complex Carbides $SC_3[TM(C_2)_2]$ (TM = Mn, Fe, Co, Ni)
15:40 – 16:00	U. Pietsch	New possibilities for time-resolved x-ray diffraction studies

16:00 – 16:05	*Time for Discussion*	
16:05 – 16:25	O. Schmidt	X-Ray Diffraction Study of the Electric Field-Induced Internal Strain in Piezoelectric $Li_2SO_4*H_2O$ and $Li_2SeO_4*H_2O$ Crystals
16:25 – 16:45	U. Wedig	Multiple Minima on the Energy Landscape of Elemental Zinc
16:45 – 16:50	*Time for Discussion*	
16:50 – 17:15	**Coffee Break**	
17:15 – 17:35	J. Henn	Practical Applications of Residual Density Analysis
17:35 – 17:55	G. Eickerling	Relativistic Effects on the Topology of the Electron Density
17:55 – 18:00	*Time for Discussion*	
18:00 – 20:00	**Poster-Session**	
21:15 – 23:00	**Concert (XVth Century Vocal Music) Polyphonic Choir "Le Voci del Mesma"**	

Sunday, June 8		
09:00 – 09:50	**P. Luger**	**KN 9: Experimental Electron Density Work in the Life Sciences: From Small to Macromolecules**
09:50 – 10:10	R. Kalinowski	Comparative Charge Density Study on Tripeptides of The Type ALA-XXX-ALA
10:10 – 10:30	T. Schirmeister	Electron Density Determination and Quantum Chemical Computations of Protease Inhibitor Model Compounds: Prediction of Reactivity
10:30 – 10:35	*Time for Discussion*	
10:35 – 11:00	**Coffee Break**	
11:00 – 11:20	R. F. Fink	Influence of Enzymatic Environments of Inhibitor Densities: Epoxide E64C Related Compounds in Cathepsin B
11:20– 11:40	S. v. Smaalen	Charge Density in Hydrogen Bonds By the Maximum Entropy Method
11:40 – 12:00	M. Kaupp	QTAIM and ELF Studies of Polar Metal-Ligand Bonds
12:00 – 12:10	*Time for Discussion*	
12:10 – 12:40	**V. Barone**	**KN 11: Spin density and magnetic properties of organic free radicals**
12:40 – 14:00	**Lunch**	
14:00 – 20:00	**Social Tour:** Boat tour on the Lake Como leaving from Gravedona; visit of the Abbey of Piona and Villa Monastero in Varenna; ECDM5 welcome cocktail at Hotel Victoria in Varenna; boat tour and return to Gravedona	

Monday, June 9		
09:00 – 09:50	**B. B. Iversen**	**KN 10: Application of synchrotron charge densities in material chemistry**
09:50 – 11:10	**ECDM5-MS3** Large facilities and charge density in the life sciences **chair: J. Helliwell**	09:50 – 10: 20 **Jonathan Wright** Accurate low resolution data for proteins from powder diffraction 10:20 – 10:45 **Slawomir Domagala** Generalization of the experimental multipolar pseudo-atom library 10:45 – 11:10 **Stefan Mebs** Charge density of B12-vitamins
11:10 – 11:35	**Coffee Break**	
11:35 – 12:50	**ECDM5-MS2** Charge, Spin, and Momentum densities in Materials Science **chair: Y. Wang**	11:35 – 12:00 **Masaki Takata** The MEM charge density and electrostatic potential study with nano-applications 12:00 – 12:25 **Alessandra Forni** Halogen Bonding interaction: investigation through charge density studies and applications in the design of new functional materials 12:25 – 12:50 **Wolfgang Jauch** Charge density in Ferromagnetic Iron and Nickel from Gamma-ray diffraction
12:50 – 14:30	**Lunch**	
14:30 – 15:20	**A. Gavezzotti**	**KN 6: Charge density and intermolecular potential. Towards a theory of molecular aggregation and crystallization**
15:20 – 16:10	**P. Coppens**	**KN 7: Intermolecular interactions: a multipolar model approach**

16:10 – 16:30	**Coffee Break**	
16:30 – 18:30	**ECDM5-MS7** Molecular interactions: the charge density viewpoint **chair: M. Spackman**	16:30 - 16:50 **Mark Spackman** Intermolecular interactions in molecular crystals: hydrogen bonding or crystal field effects? 16:50 - 17:20 **Enrique Espinosa** The relevance of the topological analysis of the electrostatic potential in molecular interactions 17:20 - 17:40 **Bartolomeo Civalleri** B3lyp augmented with an empirical dispersion term as applied to molecular crystals 17:40 - 18:00 **Kersti Hermansson** Electron density maps help explain O-H vibrational frequency shifts 18:00 - 18:15 **Jan-Peter Klöckner** Investigations on the nature of H---H bonding interactions in co-salophene complexes 18:15 - 18:30 **Yulia Nelyubina** Anion-anion interactions in ionic crystals
18:30 – 20:00	**Poster-Session**	

Tuesday, June 10		
09:00 – 09:50	**A. Martín Pendás**	**KN 1: Long live the QTAIM. New ideas in the Quantum theory of Atoms in Molecules**
09:50 – 11:05	**ECDM5-MS4** New functions and descriptors for chemical bonding **chair: M. Kohout**	09:50 – 10:25 **Frank Wagner** Topological Decomposition and Reconstruction of the Electron Localizability Indicator 10:25 – 10:45 **Hugo J. Bohorquez** The local representation of observables: toward a unified theory in quantum chemistry? 10:45 – 11:05 **Alberto Otero de La Roza** Evolution of the electron density flatness along the Periodic System
11:05 – 11:30	**Coffee Break**	
11:30 – 13: 00	**ECDM5-MS6** Static and dynamical aspects of charge density **chairs: R.F.W. Bader and C. Matta**	11:30 – 12:05 **Lou Massa** The transition state for formation of the peptide bond in the ribosome 12:05 – 12:40 **Mark Eberhart** Bonds in molecules 12:40 – 13:00 **Fernando Cortes-Guzman** Structural and bond evolution in organic reactions mechanisms
13:00 – 14:40	**Lunch**	
14:40 – 15:30	**B. Dittrich**	**KN 5: Including theoretical information for obtaining additional and more reliable information from X-ray diffraction data**
15:30 – 17:00	**ECDM5-MS5** New directions in charge density refinement and density matrix reconstructions (*in memory of Niels Hansen*) **chair: F. Larsen**	15:30 – 16:00 **Claude Lecomte** From minerals to proteins: a review of success and pittfalls of the mutipolar atom refinement 16:00 – 16:30 **Jean Michel Gillet** Making possible the refinement of reduced density matrices 16:30 –17:00 **Tibor Koritsanszky** Charge Density Refinements using the Standard and Upgraded Pseudoatom Model

17:00 – 17:20	**Coffee Break**	
17:20 – 18:00	**Additional ECDM5-MS**	Sponsor presentations 17:20 –17:40 **Zoltán Gál** Combining the high-sensitivity, fast duty-cycle Atlas CCD camera with a sub 15K Helijet in applications for charge density measurements. 17:40 –18:00 **Leo Straver** *t.b.a.* 18:00 –18:15 **Jurgen Graf** Small X-ray beams for small crystals: pushing the limits of home-lab x-ray sources
18:00 – 19:30	**Poster-Session**	
19:30 – 24:00	**Social Dinner:** 19.30 departure for restaurant “Il Beccaccino” (Sorico); 20.30-23.00 Dinner ; 23.00 Departure from the Restaurant to Gravedona	

Wednesday, June 11		
09:00 – 09:50	**R. Dovesi**	**KN 3: The role of charge and spin density in the quantum mechanical simulation of crystalline solids. The case of $X_3Y_2Si_3O_{12}$ garnets.**
09:50 – 10:40	**M. I. Eremets**	**KN 4: Chemistry of simple molecular systems at high pressure**
10:40 – 11:45	**Brunch**	
11:45 – 13:00	**ECDM5-MS1** Chemical bonding in extreme environments: Crystallography under high pressure or electric field **chair: U. Pietsch**	11:45 – 12:20 **S. Gorfman** Crystallography under external electric field 12:20 – 12:40 **Nicola Casati** The effects of high pressure on soft chemical interactions. 12:40 – 13:00 **Richard Weihrich** AIM study of halfantiperovskites $ANi_{3/2}S$ (A = In, Pb)
13:00 – 13:30	**Closing Ceremony**	
13.40	Departure from Gravedona to Milan airports (Arrival at Malpensa or Linate approx. at 16:00)	