ISAMS2014 School Programme

Registration is scheduled on Sunday, July 20th at 16.00 at Vitus (Hinter der Grieb 8, City center, GPS 49.0188307,12.0949587)

Sunday 20th	Regensburg City
16.00 - 17.00	Registration: Vitus (Hinter der Grieb 8, City center, GPS 49.0188307,12.0949587)
17.00 - 17.15	Opening remarks and Welcome addresses (***R. Weihrich***)
17.15 - 17.45	CRYSTAL14: New features overview (***R. Dovesi***)
17.45 - 18.45	Participants self-introduction (one-slide/one-minute presentation)
18.45 - 20.30	Welcome Party: Vitus (Hinter der Grieb 8, City center)

Morning Sessions - H47, Department of Chemistry (University of Regensburg)

	Monday 21st	Tuesday 22nd	Wednesday 23rd	Thursday 24th	Friday 25th
8.30 - 9.15	Translation symmetry, Space groups, Bloch functions, Fermi energy ***R. Orlando***	Geometry optimization and transition state search in periodic systems ***C. M. Zicovich-Wilson***	Low dimensionality systems ***B. Civalleri***	CRYSTAL in parallel: replicated and distributed (MPP) data ***R. Orlando***	Post-HF methods ***M. Schutz***
9.15 - 10.00	Hamiltonians and basis sets ***B. Civalleri***	One-electron properties ***A. Erba***	On the use of point symmetry in periodic (and molecular) SCF calculations ***C. M. Zicovich-Wilson***	Chemistry at spin centers ***M. Peintinger***	CRYSCOR project ***D. Usvyat***
	Coffee Break	*Coffee Break*	*Coffee Break*	*Coffee Break*	*Coffee Break*
10.30 - 11.15	Consistent Gaussian Basis Sets for Solid-State Calculations ***M. Peintinger***	Electronic structure: electrons in momentum space ***U. Wedig***	Dielectric properties with CRYSTAL ***R. Orlando***	Dielectric properties with CRYSTAL (II) ***R. Orlando***	The energy landscape concept ***A. Krach***
11.15 - 12.00	Structure of the CRYSTAL code ***R. Dovesi***	Beyond band structure and DOS: tensorial properties of crystals ***A. Erba***	Vibrational frequencies of solids: Lattice dynamics and phonon dispersion ***K. Doll***	Bonding in direct space: ELF, AIM ***R. Weihrich***	Nucleation and phase transitions ***P. Ectors (Zahn)***
12.00 - 12.45	CRYSTAL input/output. Basic features ***B. Civalleri***	Some steps in solid solutions ***P. D'Arco***	Simulation of IR/RAMAN spectra ***R. Dovesi***	Models and strategies for metallic systems: bulk and surfaces ***K. Doll***	Final remarks and future challenges ***A. Pfitzner***

Afternoon Sessions - Linux Pool, Department of Chemistry, UR

Basic tutorials (Non CRYSTAL users)

	Monday 21st	Tuesday 22nd	Wednesday 23rd	Thursday 24th	Friday 25th
14.30 - 16.15	Geometry input & Basis sets	Geometry optimisation	*Poster Session Chemistry Department - Univ. Regensburg*	Vibrational frequencies	Basic modelling of surfaces and defects
	Break	*Break*		*Break*	*Break*
16.45 - 18.30	Total energy (Single-point calculation)	EOS		One-electron properties	Free hands-on tutorials

Advanced tutorials (CRYSTAL users)

	Monday 21st	Tuesday 22nd	Wednesday 23rd	Thursday 24th	Friday 25th
14.30 - 16.15	Advanced options in geometry optimisation	Solid solutions	*Poster Session Chemistry Department - Univ. Regensburg*	Advanced options in vibrational frequencies calculation	CRYSCOR
	Break	*Break*		*Break*	*Break*
16.45 - 18.30	EOS	Tensorial properties		Dielectric properties	Free hands-on tutorials

Social events

	Monday 21st	Tuesday 22nd	Wednesday 23rd	Thursday 24th	Friday 25th
			17.30 *Guided city tour: Regensburg (Meeting point: Historische Wurstkuchl GPS: 49.020971,12.097735 Thundorfer StraÃŸe)*	19.00 *Social Dinner: □lte Linde Muellerstrasse 1, 93059 Regensburg GPS 49.02302,12.095517 Tel.: +49-941-88080*	