PROGRAM COST D37 PRAGUE MEETING
APRIL 7 TO 9, 2009
(DRAFT 24.2.)

TUE, APRIL 7, 2009

REGISTRATION

WELCOME (Jiri Pittner)

PART A: WORKING GROUP MEETINGS (PRIVATE)

TUE, APRIL 7, 2009

WG01: 5 Presentations (2hrs30min)

WG02/03: 2 Presentations plus General Discussion (2hrs30min)

WG04: 2 Presentations plus General Discussion (2hrs 30 min)

WG05: no WG meeting

Part B: JOINT WG-MEETING (PUBLIC / PLENARY)

TUE, APRIL 7, 2009

		SPEAKER	TITLE	WG
16:00	16:30	G. Lendvay	*A survey of approximate dynamical methods for Large Systems*	02/ 03
16:30	17:00	A. Benscura	*Restructuring the ABC quantum reactive scattering code for Grid applications and deployment*	02/ 03
17:30	18:00	S. Rampino	*The time independent ABC code as a case study for quantum dynamics data models and standards*	02/ 03
18:00	18:30	A. Saracibar	*The time dependent RWAVEPR code for quantum dynamics calculations of detailed reactive probabilities*	02/ 03

WED, APRIL 8, 2009

		SPEAKER	TITLE	WG
08:30	09:00	Peter G. Szalay	*Excited Electronic States of Cytosine: the Role of Non-adiabatic Effects*	01
09:00	09:30	Jiri Pittner	*Molecular dynamics with surface hopping based on overlaps of TDDFT response functions*	01
09:30	10:00	Natasha Trendafilova	*Present status of the utilization of computational chemistry molecular modeling and simulations methodologies in Bulgaria*	01
10:00	10:30		COFFEE_BREAK	
10:30	11:30	Satoshi Sekkiguchi	TITLE OPEN	INV
11:30	12:00	Matthias Ruckenbauer	*Efficient Use of Webservices Interactively and in Complex Workflows*	01
12:00	12:30	Zvonomir Maksic	*Acidity and Basicity of Amino-acids in Water – New Advances*	01

Lunch Break

		SPEAKER	TITLE	WG
14:00	14:30	Stefano Evangelisti	*The State-of-the-Art of the DeciQ Working Group*	04
14:30	15:00	Kenneth Ruud	*Building Quantum Chemistry Programs by Divide and Conquer*	04
15:00	16:00	Ludek Matynska	TITLE OPEN	INV
16:00	16:30		COFFEE_BREAK	
16:30	17:00	Peter Murray-Rust	*Repositories for Computational Chemistry Based on CML and RDF*	05
17:00	17:30	Hans P. Lüthi	*The Properties of Donor-Acceptor Susbstituted Polyacetylenic Compounds*	05
17:30	18:00	Stefan Borini	*The COST Molecular Annotation Project: a Molecular Database Initiative for Data Mining*	05
18:00	18:30	Antonio Márquez-Cruz	*Modelling the Reactivity at Solid Surfaces: a Workflow Scenario*	05

THU, APRIL 9, 2009

		SPEAKER	**TITLE**	**WG**
08:30	09:00	S. Farantos	*Spectroscopy and dynamics of complex systems: an implementation on the grid*	02/ 03
09:00	09:30	F. Huarte	*MCTDH: a time dependent quantum and semiclassical dynamics approach to the calculation of rate coefficients*	02/ 03
09:30	10:00	A. Rodriguez	*G-FLUXO: A workflow portal ready for Computational Chemistry*	02/ 03
10:00	10:30		COFFEE_BREAK	
10:30	11:30	M. Porrini	*Molecular dynamics graphical interface*	02/ 03
11:30	12:00	A. Lagana / O. Gervasi	*Conclusions*	02/ 03
12:00	12:30	H.P. Lüthi / J. Pittner	CLOSURE OF MEETING	