



COMPUTATIONAL THEORETICAL CHEMISTRY EUCO 2019 CONFERENCE

A. Laganà, N. Faginas Lago, A. Lombardi (Local Organizing Committee)

The 12th edition of the EuChemS Computational and Theoretical Chemistry (CTC) Division Conference will be organized in **Perugia (September 1-5, 2019)** by the group "Computing, Theory and Experiments of Dynamics and Kinetics Studies for Chemical Processes" of the [Dipartimento di Chimica, Biologia e Biotecnologie](#) (University of Perugia) and the Consortium for Computational Molecular and Materials Sciences (CMS)² (www.cms-2.org). The Keynote speakers are: C. Cappelli, D. Crawford, G. Cruciani, S. Evangelisti, P. Fernandes, W. Klopper, J.P. Piquemal, F. Ruggieri, R. Sayos, P. Szalay.

---REGISTRATION FEE in €

Early registration before 31 May 2019 FEE (member 450, non member 550, member student 300, non-member student 350, accomp. person 150) including conference dinner;

Late registration from 01 June 2019 FEE (member 550, non member 650, member student 400, non-member student 450, accomp. person 200) including conference dinner;

Two days registration FEE 400 (for TCCM student, Sept 2 (full day), Sept 3 (morning) early registration 200 and late registration 250).

---VENUE

The Conference will be held at the [Hotel GIO](#) located at walking distance from the Perugia Railway station (Fontivegge), the mini-metro station (Case Bruciate) to the town Centre and the University of Perugia main campus. *Hotel GIO can accommodate all the participants to the conference at a special rate if booking is made before August 1 and mention is made to **CTC EUCO 2019** in the booking form.* Several other hotel and B&B accommodations are available in town.

---CONFERENCE TENTATIVE TIMETABLE (see table below)

the conference will be articulated as follows:

10 regular sessions (three per day, except the last one, complemented by a poster session) devoted to computational and theoretical chemistry topics chosen by the scientific committee (the local organizing committee and the board of the CTC division chaired by P. Szalay). Each regular session will host one keynote lecture (40'), two contributed oral presentations (20' each) and some research telegrams from young researchers and students (10' each) selected by the scientific committee.

5 parallel sessions of 10' oral presentations by TCCM (theoretical chemistry and computational modelling) students on Monday (all day) and Tuesday (morning) to follow the keynote talks.

1 training parallel event (open also to TCCM students) on the use of both the echemtest[®] e-tests in a cloud environment for assessing chemistry competences and the glorep distributed repository of learning objects.

---**AFTER CONFERENCE WORKSHOP on the Open Molecular Science Cloud project** (see table below Half-day (Thursday afternoon) at the headquarters of the "Accademia delle Scienze" in Rome for potential partners of the Open Molecular Science Cloud project (ad hoc bus connection from hotel GIO at 11:30 sharp)

---PUBLICATIONS and GENERAL ASSEMBLY

Accepted abstracts of orals and posters will be published by the e-magazine VIRT&L-COMM (member of the Open Journal System) at no charge. On Thursday morning (10:20-11:00) after the regular Session started at 8:20 General Assembly of the participants to discuss the policies of the CTC Division.

---TOURS

VIRT&L-COMM.15.2018.6

Guided walking tour of the city, visits to the Etruscan-Roman foundations of the Cathedral (<http://www.cattedrale.perugia.it/>) and to the Galleria Nazionale dell'Umbria can be booked at the conference desk (<http://www.artiumbria.beniculturali.it/index.php?en/1/home>). Excursion to Assisi, Spoleto, Orvieto, Norcia, Trasimeno Lake, etc. could also be arranged

---TRAVEL

There are direct flights connecting the small Perugia airport "San Francesco" (<http://www.airport.umbria.it/en/>) to London Stansted, Brussels and Frankfurt. The best option, however, is to fly to Fiumicino and take from the Rome stations (Termini or Tiburtina) a train to Perugia (<http://www.trenitalia.com/tcom-en>). There are also regular bus connections Fiumicino-Perugia (<http://www.sulga.eu/libreria/fiumicinoroma.pdf>).

---PROJECT WORKSHOP

The last day of the Conference a direct bus ride to the Accademia delle scienze arranged for the participants to the Project meeting: "Open Molecular Science Cloud" at 11:30 for departure from Hotel GIO (expected travel time is 2.0 hours, booking is requested).

	Monday 02	Tuesday 03	Wednesday 04	Thursday 05	
08:20-08:50 08:50-09:00	REGISTRATION OPENING			K10: Biochemistry (P. Fernandes)	
09:00-09:40	K1: General theory issues (P. Szalay)	K4: Electronic structure and strong correlation (W. Klopper)	K7: HPC for Photochem. and MD (D. Crawford)	O19 O20	
09:40-10:00	O1 TCCM1-2	O7 TCCM 25-26	O13	RT37-RT38	
10:00-10:20	O2 TCCM 3-4	O8 TCCM 27-28	O14	RT39-RT40	
10:20-11:00	RT1-RT4 TCCM 5-8	RT13-RT16 TCCM 29-32	RT25-RT28	GEN. CTC ASSEMBLY	
11:00-11:20 coffee break				
11:20-12:00	K2: Open Molecul. science cloud, Distr. computing (F. Ruggieri)	K5: Machine learning, Cheminformatics, QSAR (G. Cruciani)	K8: Force Fields (J.P. Piquemal)	DISPERSAL Rented bus to ACCADEMIA XL and FIUMICINO AIRPORT (to book)	
12:00-12:20	O3 TCCM 9-10	O9 TCCM 33-34	O15		
12:20-12:40	O4 TCCM 11-12	O10 TCCM 35-36	O16		
12:40-13:20	RT5-RT8 TCCM 13-16	RT17-RT20 TCCM 37-40	RT29-RT32		
13:20-14:30	LUNCH				
14:30-15:10	K3: Catalysis (R. Sayos)	K6: Spectroscopy (C. Cappelli)	E-tests, Learning Objects (S. Evangelisti)	FROM 2PM ON PROJECT MEETING OPEN MOLECULAR SCIENCE CLOUD at ACCADEMIA DELLE SCIENZE (ROME)	
15:10-15:30	O5 TCCM 17-18	O11 Training on Echemtest	O17		
15:30-15:50	O6 TCCM 19-20	O12	O18		
15:50-16:10	RT9-RT12 TCCM 21-24	RT21-RT24	RT33-RT36		
16:10-18:30	coffee break + poster session	Ch + poster session CTC Board meeting	Training on CTC Board meeting		coffee break + poster session CTC Board (meeting contin.)
18:30	Welcome party	TOURS: National gallery (to book) or Etrusc/roman Cathedr. found (to book)			
20:30				CONF. DINNER (to book)	