



COMPUTATIONAL THEORETICAL CHEMISTRY EUCO 2019 CONFERENCE

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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 following Keynote speakers have already accepted the invitation: C. Cappelli, G. Cruciani, D. Crawford, S. Evangelisti, P. Fernandes, W. Klopper, J.P. Piquemal, F. Ruggieri, R. Sayos.

---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

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
08:20-09:00	REGISTRATION & OPENING			K10: Biochemistry/ Astrochemistry
09:00-09:40	K1: General theory issues	K4: Electronic structure and strong correlation	K7: Nuclear dynamics and Photochemistry	O19
09:40-10:00	O1 TCCM1-2	O7 TCCM 25-26	O13	O20
10:00-10:20	O2 TCCM 3-4	O8 TCCM 27-28	O14	RT37-RT38
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 Molecular science, Supercomputing	K5: Machine learning, Cheminformatics, QSAR	K8: Force Fields	Rented buses 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	K6: Spectroscopy E-tests, Learning Obj	K9: Solid state and Materials	FROM 2PM ON PROJECT MEETING OPEN MOLECULAR SCIENCE CLOUD ACCADEMIA NAZIONALE DELLE SCIENZE (del XL) 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	
16:30-18:30	coffee break + poster session 1	coffee break + poster session 2 CTC Board meeting	Training on LO repository coffee break + poster session 3 CTC Board (meeting contin.)	
18:30	Welcome party	TOURS: National gallery (to book) or Etruscan/roman Cathedral foundations (to book)		
20:30			CONF. DINNER (to book)	