The EuChemS Computational and Theoretical Chemistry Division Conference and the Open Molecular Science Cloud Workshop

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During the 7th EuCheMS Congress "Molecular frontiers and global challenges" (Liverpool (UK) August 26-30, 2018) [1], the CTC (Computational and Theoretical Chemistry) Division held the Symposium "*Methods of computational chemistry: challenges and new developments"*. At the Symposium it was agreed that the CTC (Sept 1-5 2019) European Conference (EUCO 2019) going to be held in Perugia (IT) would be run jointly with an Open Molecular Science Cloud (OMSC) Workshop supported also by the US Molecular Sciences Software Institute (MolSSI) and the Accademia delle Scienze detta dei XL of Rome where the final sessions would be held. There it was also decided that related invited Lectures:
1) Péter G. Szalay, *General theory issues,*
2) Stefano Evangelisti, Estefania Alves Alves, Gian Luigi Bendazzoli, and Arjan Berger, *Clifford boundary conditions for periodic systems,*
3) Ramón Sayós, Hèctor Prats, Sergio Posada-Pérez, José A. Rodriguez and Francesc Illas *First-principles-based kinetic Monte Carlo simulations in heterogeneous catalysis: Application to water-gas shift reaction with several catalysts,*
4) Wim Klopper, *Bethe–Salpeter correlation energies of atoms and molecules,*
5) Gabriele Cruciani, *Computational chemistry and artificial intelligence,*
6) Chiara Cappelli, *Fully atomistic embedding approaches for the computational spectroscopy of complex systems: status and perspectives,*
7) Daniel G. A. Smith, *Advancing the computational molecular sciences through better theory and better software,*
8) Jean-Philip Piquemal, *Scalable polarizable molecular dynamics using Tinker-HP,*
9) Federico Ruggieri, Fulvio Galeazzi, Federica Tanlongo, *European Open Science Cloud and the EOSC-Pillar Project,*
10) Pedro Alexandrino Fernandes, *Dynamic and chemical disorder in enzymatic reaction mechanisms.*
(see also [2]) would be published in Vitrt&l-Comm.

In partial parallelism with the CTC EUCO 2019, the OMSC workshop was held during the days 3-6 of September. The name of the speakers and the title of their presentations at the workshop are given below and related abstracts are also given in the present issue of the e-magazine.

♦ **Sept 3**

Osvaldo Gervasi, Sergio Tasso, and Antonio Laganà, *Open molecular science cloud educational tools for chemistry: LibreEOL and G-Lorep training and coaching event*
Osvaldo Gervasi, Antonio Laganà, and Sara Tortorella, *Open learning and innovative didactics of chemistry in EChemTest®*

♦ **Sept 5**

Giuseppe Vitillaro, and Edoardo Mosconi, *Open molecular science cloud photovoltaic training demo on VHerla*
(from here on continued in Rome at the Accademia delle Scienze detta dei XL with an extended replica of the Lectures 7-9 mentioned above) plus:
Antonio Laganà, Giuseppe Vitillaro, and Ernesto Garcia, *The Molecular simulator enabled cloud services: MOSEX*

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Edward Blurock, *Cloud services for reaction modeling*
Moises Álvarez-Moreno, and Carles Bo, *ioChem-BD: tools for open-access publishing and much more …*

♦ **Sept 6**

Vinícius Wilian D. Cruzeiro, *Possible applications for the Open Molecular Science Cloud: AMBER simulations and development of highly accurate many-body potentials*
Grier_M._Jones, *Cloud Computing ideas on European Open Science Cloud (EOSC)*
Jessica Maat, *Data Driven Parameterization of Force Fields*
S. Seritan, and T.J. Martinez, *Nonadiabatic Dynamics Study of the B850-B800 Complex in LH2 using TeraChem Cloud.*

The presentations ended with a discussions on the design of the MOSEX (Molecular Open Science Enabled Cloud Services) project for the production, validation and re-use of Molecular Science (MS) data on the cloud, their articulation in electronic structure and equilibrium molecular configurations, reactive and non reactive dynamics, design of bioactive molecules, management of distributed repositories and dissemination, publication, evaluation and validation of molecular knowledge.
To this end the following strategic lines were singled out in order to coordinate joint actions:

- **a. PRODUCING/DISCOVERING/ACCESSING/DOWNLOADING:** MS data set(s)
- **b. RUNNING/CHECKING/TERMINATING/VALIDATING:** MS data set(s)
- **c. ANNOTATING/CURATING/PRESERVING:** specific MS data set(s)
- **d. EVALUATING AND REWARDING THE QUALITY OF PROVIDED SERVICES**

and

♦ **Services**

a) SERVICE 1: PRODUCE/DISCOVER and DOWNLOAD MS DATA

- The main service will consist in operating OPEN COLLABORATIVE and FULLY RE-USABLE DATABASES and REPOSITORIES (like the above mentioned ioCheM-BD, CHEMCONNECT, QCArchive) of FAIR (Findable, Accessible, Inter-operable and Re-usable) validated data by producing/discovering/accessing/downloading so as to enhance TOP (Transparency and OPenness) MS knowledge through the promotion of good scientific practices of accountability, traceability and reproducibility.

b) SERVICE 2: RUN/CHECK/TERMINATE/VALIDATE

- The provision of SERVICE 1 will lever collaborative run, check, terminate and evaluate iterative operations (collaboratively provided by the members of the MS community) aimed to validate MS data by comparing results obtained by different users adopting different computational tools.

c) SERVICE 3: ANNOTATE/CURATE/PRESERVE

- The Data validated by SERVICE 2 will be properly annotated and curated for preservation and more efficient re-use according to the standards adopted by the EOSC-Pillar initiative. The development of appropriate tools for their efficient re-use will be of invaluable help for further research and applications by public institutions and private companies.

d) SERVICE 4: QUALITY OF SERVICE EVALUATION

- The general organization of the project, its articulation in WGs and the outcomes of services (a), (b) and (c) provided by the members of the MS community will be evaluated using QoS (quality of service) techniques while users will be profiled using QoU (quality of users) techniques.

e) SERVICE 5: THE PROSUMER MODEL OF DEBITS/CREDDITS OFFSETTING

- The community model adopted is inspired to the Prosumer (Producer+Consumer) one (as already implemented for EChemtest®[3]) in which the community members are at the same

time users (making debits for used services) and producers (gaining credits for produced services) of cloud services. Among the members of the community there will some Market spinners taking care of offering auxiliary paid services to external users whose net gains will be invested in the community activities and development.

- **Thematic areas**

a) THEMATIC AREA 1: ELECTRONIC STRUCTURE, SPECTROSCOPY, PHOTOCHEMISTRY, PHOTOVOLTAIC.

GOAL: importing, producing, analysing, validating and making freely available for re-use data on:

- high level electronic structure calculations
- molecular structures-properties relationships
- electronic structure evolution in chemical transformations

APPLICATIONS: molecular properties, innovative materials, excited electronic states processes.

b) THEMATIC AREA 2: EFFICIENCY OF GAS PHASE PROCESSES

GOAL: importing, producing, analysing, validating and making freely available for re-use data on:

- full range potential energy surfaces and data driven qc
- cross sections and rate coefficients of elementary processes
- rates of complex gas, surface and condensed phase processes

APPLICATIONS: astrochemistry, combustions, energy storage, catalysis, polarizable molecular dynamics.

c) THEMATIC AREA 3: MACRO-BIO-PHARMA PROPERTIES AND PROCESSES

GOAL: importing, producing, analysing, validating and making freely available for re-use data on bio and pharmaceutical molecules:

- structures: docking cavities characterization
- processes: md simulations of biomolecules
- properties: artificial intelligence determination
- properties: virtual screen lead identification and optimization

APPLICATIONS: de novo design of drugs, biomolecules, nutriceutics.

d) THEMATIC AREA 4: MS KNOWLEDGE DISSEMINATION

GOAL: importing, producing, analysing, validating and making freely available chemical knowledge through:

- open e-magazine publication
- learning objects and multimedia products
- e-assessment g-lorep, demo-echemtest

APPLICATIONS: chemical knowledge diffusion, multimedia supported open learning, e-assessment and certification.

References

1] https://www.euchems2018.org/
2]http://web.chm.unipg.it/chimgen/mb/theo2/EUCO2019/EUCO2019/Welcome_files/Book%20of%20abstracts.pdf
3] A. Laganà, O. Gervasi, S. Tasso, D. Perri, F. Franciosa, The ECTN Virtual Education Community prosumer model for promoting and assessing chemical knowledge, Lecture notes comput science 10964, 533-548 (2018), DOI: 10.1007/978-3-319-95174-4_42; ISBN 978-3-319-95167-6