MOSEX: MOLECULAR OPEN SCIENCE ENABLED CLOUD SERVICES

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1-PREAMBLE

At the recent (September 2019, University of Perugia (PG, IT) and Accademia Nazionale delle Scienze detta dei XL (Rome, IT)) Open Molecular Science Cloud (OMSC) Workshop, we launched the Molecular Open Science Enabled Cloud (MOSEX) project aimed at establishing a cloud service for validating the value of the rate coefficient parameters of elementary chemical processes via an iterative synergistic use of theory and experiments. In order to implement MOSEX we assembled an international team of molecular scientists and we activated links with the NFDI4Chem (DE) and the MolSSI (US) consortia of research data infrastructures for molecular science (MS). At the same time we established an OpenStack platform (Herla) at our CNR Institute extended to the Department of Chemistry, Biology and Biotechnology (DCBB) of the University of Perugia within the CMS^2 Consortium [1]. Later its cloud image (VHERLA) was experimentally implemented at the GARR Cloud [2] node of Palermo as a Virtual Data Centre.

2-THE GOALS OF THE MOSEX PROJECT

VHerla MOSEX services will be specialized to:

a) produce/discover/access/download,
b) run/check/terminate improper results/validate,
c) annotate/curate/preserve,

data inherent to elementary molecular processes when satisfactorily convergenced.
Initial activities in this respect trace back to D23 METACHEM [3] and D37 GRIDCHEM [4] Actions of COST [5] and within COMPCHEM VO [6] and CMMST VRC [7] activities of the EGEE III [8] and EGI Inspire [9] EU initiatives. Here its evolution is proposed for insertion into the European Open Science Cloud (EOSC) [10] Pillar Initiative. This will provide OMSC with the ideal cloud breath necessary to overcome the current limits and fragmentation of molecular science research and technologies in the field.
More precisely, MOSEX will gather together the world top competences of its members in:
1. electronic structure and equilibrium molecular configuration properties methods and computational techniques for spectroscopy, synthesis, photovoltaic and photochemical processes;
2. quantum, quantum-classical and classical methods and computational techniques for reactive and non reactive efficiency studies for elementary and complex detailed kinetics;
3. structure-property relationships approaches to the determination of the properties of more complex (combustion, materials, energy conversion, etc.) systems;
4. management of distributed repositories and databases for chemical systems [11-13];
5. dissemination, publication and assessment of molecular knowledge: e.g. EChemtest® e-tests, VIRT&L-COMM e-magazine, G_LOREP Learning objects [14].
The various steps will be specialized as follows:

- **a)** *producing/discovering and downloading* MS data for the open collaborative and fully re-usable databases and repositories. For this purpose CHEMCONNECT [11], ioCheM-BD [12] and QCArchive [13] open databases of FAIR (Findable, Accessible, Inter-operable and Re-usable) validated data enhancing TOP (Transparency and OPenness) MS knowledge are used by promoting good scientific practices of accountability, traceability and reproducibility;
- **b)** *running/checking/correcting (where possible) or discarding and validating* data of service (a) through iterative cycles collaboratively undertaken by the members of the community for the validation of MS data by comparing results obtained by different users when adopting different computational tools;

ISSN: 2279-8773

- **c)** *annotating/curating/preserving* data of service (b) for a 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 in order to further enhance research and applications by public institutions and private companies;

The above steps will act as a support not only to the research work of the European Division of Computational and Theoretical Chemistry but will also provide support to the Materials, Astrochemistry, Combustion, Circular economy, etc. application fields. Additional features to be implemented in MOSEX are:

- **d)** *evaluating the quality of services* (a), (b) and (c) provided by the members of the MS community will be evaluated using QoS (quality of service) techniques while the users will be profiled using QoU (quality of users) techniques [15];
- **e)** *offsetting debits with credits of the adopted Prosumer (Producer+Consumer) model* already implemented on the cloud by the European Chemistry Thematic Network for the electronic assessment EChemtest® product [14] in which the community members are at the same time users (accumulating debits for used services) and producers (gaining credits for produced services) with the help of a Market spinner for the provision of paid services (http://ectn.eu/committees/virtual-education-community/echemtest/).

3-TEAMS AND LINKS [16]:

the University of Perugia (the Department of Chemistry, Biology and Biotechnologies and the Department of Mathematics and Computer Science) and the Perugia section of the CNR SCITEC Institute;

the European Research Institutions: Laboratory de Chimie Theorique (Sorbonne University), the Institute of Chemical Research of Catalonia (Tarragona), the Department of Pharmacy, University of the Basque Country (Vittoria);

the NFDI4Chem - Chemistry Consortium for the National Research Infrastructure

the US Molecular Science Software Institute MolSSI (Blacksburg);

the Companies: Molecular Horizon srl (Bettona), the Master-UP srl (Perugia), the Blurock Consulting AB (Lund).

4-E-INFRASTRUCTURE TASKS

Provide the relevant repository of validated data of low temperature rate coefficients of Chemical reactions from comparison of experiments and accurate dynamical calculations;

Provide the relevant repository with some estimates of high temperature rate coefficients for combustion validated by comparing experiments and accurate dynamical calculations;

Provide the relevant repository with some estimates of properties of Photovoltaic materials validated by comparing experiments and accurate electronic structure calculations

Provide the relevant repository with some Chemical knowledge Learning objects (LO)s[17]. and the EChemTest® Self-evaluation assessment tests run in joint operations of public institutions and private companies based on the Prosumer model

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