1) Antonio Laganà
Open Molecular Science and welcome to the OSC School

The Open Science Cloud project is at present getting off the ground within EINFRA 12 (a) under the joint action of EGI.eu, INDICO and EUDAT. The molecular science community is not among the direct players of the project even if the COMPCHEM Virtual Organization and the CMMST (Chemistry, Molecular & Materials Science and Technologies) Virtual Research Community (VRC) are since long operating in the field (see https://www.egi.eu/use-cases/research-stories/) of Open Molecular Science thanks also to a tight connection with colleagues from Physics. As a matter of fact, this school funded by the European doctorate in Theoretical Chemistry and Computational Modelling (TCCM) TN-EJD-642294_TCCM is being jointly run by the Department of Chemistry, Biology and Biotechnologies and the Physics Department and some of the applications that will be illustrated during the school are based on a common cloud Openstack infrastructure. After all, I must admit that my first moves in distributed and cloud computing were fostered by some joint initiatives with INFN friends.

However, an Open Molecular Science Community is at present still a dream and its realistic objective is to foster the conversion of the present attitude of the Molecular Science Community to act largely as a scattered ensemble of isolated “islands” into a collaborative “continent” by building a collaborative management of computational tools and data covering the whole lifecycle of Molecular Science knowledge using metadata, ontologies and provenance based on advanced data and computing services. The initiative will incorporate as stakeholders research facilities, technology providers, research teams and SMEs for the purpose of:

1. gathering together the researchers and companies running simulations in Computational and Experimental Chemistry within a network of European, regional and national research facilities and e-infrastructure resources and services;

2. ensuring intuitive, seamless and virtual access to key European, regional and national research facilities and e-infrastructure resources and services considering different levels of expertise and skills of the members;

3. supporting efficient management of scientific data including creating, publishing, accessing, curating, preserving data using metadata, ontologies and provenance based on advanced data and computing services;

4. enabling and supporting multi-disciplinary activities in cooperation with ESFRI and other major European initiatives to address societal challenges.

Of all this the present school intends to be a key step by training the first European coort of Theoretical Chemistry and Computational Modeling PhD.