

## Open Molecular Science Cloud Photovoltaic training Demo on VHerla

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Within the innovative collaborative approach to Computing and Data infrastructures [1] adopted by the European Open Science Cloud (EOSC) [2] Pillar Project, the articulation and the usage of VHerla (a cloud platform activated at the Dipartimento di Chimica, Biologia e Biotecnologia (DCBB) of the University of Perugia, and later extended to the CMS<sup>2</sup> Consortium of DCBB (CNR ISTM - UOS Perugia plus Master-UP srl and Molecular Horizon srl), to the Dipartimento di Matematica ed Informatica (DMI), to the Dipartimento di Fisica e Geologia (DFG), and to INFN Perugia), will be illustrated for training purposes. In particular, the VHERLA evolution (the cloud image of the Perugia OpenStack platform devoted to the activities of the CMS<sup>2</sup> Molecular Sciences consortium (<http://www.cms-2.org/index.php>) implemented as a Virtual Data Center within the GARR (<http://www.garr.it/b/eng>) Cloud [4] at the node of Palermo, will be discussed and services offered to the relevant community analyzed.

Among the planned applications of the project a photovoltaic one in the field of a new generation of materials (via the computational investigation of Dye Sensitized and Perovskite Solar Cells using DFT, TDDFT, ab initio Car–Parrinello molecular dynamics and GW methods to predict and interpret the optical and electronic properties of materials and interfaces [5,6]) will be illustrated for training purpose.

### References

- 1] European Cloud Initiative - Building a competitive data and knowledge economy in Europe, Brussels, 19.4.2016 COM(2016) 178 final - COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT, THE COUNCIL, THE EUROPEAN ECONOMIC AND SOCIAL COMMITTEE AND THE COMMITTEE OF THE REGIONS
- 2] <https://www.eosc-portal.eu/>
- 3] <https://aco-itn.oapd.inaf.it/>
- 4] G. Vitillaro and A. Laganà – vherla: a virtual molecular science data center allocated on the garr cloud, Virt&L-COMM 2018-12-11
- 5] "Cation-Induced Band-Gap Tuning in Organohalide Perovskites: Interplay of Spin–Orbit Coupling and Octahedra Tilting" Amat, A.; Mosconi, E.; Ronca, E.; Quarti, C.; Umari, P.; Nazeeruddin, M. K.; Graetzel, M.; De Angelis, F.; *Nano Lett.* 2014, 14, 3608–3616.
- 6] "Defects Migration in Methylammonium Lead Iodide and their Role in Perovskite Solar Cells Operation" Azpiroz, J. M.; Mosconi, E.; Bisquert, J.; De Angelis, F.; *Energy Environ. Sci.* 2015, 8, 2118– 2127.