



# EGI Community Forum 2015

## Thursday 12 November 2015

### Advances in the computational chemistry and material science field - Sala A+A1, Giulia centre (15:15-16:45)

-Conveners: Antonio Lagana

| time  | [id] title   | presenter           |
|-------|--|---------------------|
| 15:15 | [197] Virtual Research Environment and Computational Chemistry Community   | TERSTYANSZKY, Gabor |
| 15:35 | [198] Collaborative service on ab initio evaluation of gas phase processes efficiency  | LAGANA, Antonio     |
| 15:55 | [199] From ab-initio calculations to full technological systems simulations: application to aerospace and nuclear fusion                 | ESPOSITO, Fabrizio  |
| 16:15 | [200] General discussion on: Building multiscale simulations and data repositories on the efficiency of Molecular processes as a service | LAGANA, Antonio     |