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## Towards a Specialized Support Centre for chemistry and materials sciences

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### Abstract

Leading the efforts of a group of 10 European research Laboratories belonging to the Czech Republic, Finland, France, Greece, Italy, Poland, Spain, and Switzerland, UNIPGCHIM (a research group of the Department of Chemistry of the University of Perugia (I) extended to researchers of the Department of Physics and the Department of Mathematics & Informatics) has elaborated in collaboration with CYFRONET (the Academic Computer Centre of the AGH University of Science and Technology of Krakow (Pl)) a proposal for the call INFRA-2010-1.2.3 "Virtual Research Communities" to assemble a Specialized Support Centre (SSC) for Chemistry and Materials Sciences and Technologies.

The SSC is founded on the EGEE coordination activities of some Virtual organizations (like COMPCHEM, GAUSSIAN, VOCE), service activities of some of its potential members (CSC, CYFRONET, DEMOCRITOS, ENEA, NCBR, UNIPGCHIM) and research activities of FORTH, GDRQ, UZH and IRSAMC in addition to those of the previous institutions. In addition, more than hundred research laboratories have expressed their wish to exploit the support of the proposed SSC

The SSC will:

- Support its users in structuring and running their applications on the grid
- Adopt models and standards for molecular and material knowledge allowing inter- and intra- applications and platforms operability
- Implement on the grid libraries of codes and services for the users
- Design and develop tools for rewarding the efforts spent by the users to contribute to the activities of the SSC on behalf of the community

**Session Classification:** Computational Chemistry – Cluster status and evolution