

Session Program

21-25 Sept 2009



EGEE'09 - Uniting our strengths to realise a sustainable European grid

Computational Chemistry -- Cluster status and evolution

Hotel Barcelo Sants
Barcelona

Tuesday 22 September

11:00

Computational Chemistry -- Cluster status and evolution

Session | Location: Hotel Barcelo Sants, L'Eixample, Barcelona

11:00-11:25

Quantum Grid Dynamics (QGD): a method for solving the molecular Schroedinger Equation in Cartesian coordinates via angular momentum projection operators

11:25-11:50

Towards a Specialized Support Centre for chemistry and materials sciences

11:50-12:15

Virtual Organisation for Central Europe (VOCE) achievements

12:15-12:40

Current status of Chempo web portal

12:40-13:00

Grid calculation of reaction kinetic coefficients: a quantum mechanical approach

13:00