

SECOND YEAR MEETING OF THE
AUCAT FIRB 2010
PROJECT

22 July 2014
at Auditorium DCFA


9.20 Prof. Alessandro Del Zotto
University of Udine

WELCOME

9.40 Dr. Leonardo Belpassi
CNR-ISTM of Perugia
«Computational Catalysis: Past, Present and Future»

LECTURE

10.40 Dr. Gianluca Ciancaleoni CNR-ISTM of Perugia
«Relationship between Au-C bond properties and experimental observables»

11.10 Coffee Break 

11.40 Dr. Sergio Rampino CNR-ISTM of Perugia
«Charge Displacement analysis on relativistic electron densities with the Dirac-Kohn-Sham parallel program BERTHA»

12.00 Marina Trinchillo University of Napoli
«Further insights into the mechanism of the alkoxylation reaction: determination of activation parameters»

12.20 Giovanni Bistoni University of Perugia
«Is the CO stretching frequency a probe for the chemical bond in transition metal carbonyl complexes?»

12.40 Luca Biasiolo University of Udine
«Influence of the nitrogen acyclic carbene ligand (NAC) on the anion position and catalytic performance of cationic gold catalysts»

13.00 Dr. Daniele Zuccaccia
University of Udine

CONCLUDING REMARKS

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