

PUBLICATIONS ET CONGRES (septembre 2010)

✓ Articles dans des journaux internationaux à comité de lecture

[3] **S. Di Tommaso**, V. Tognetti, E. Sicilia, C. Adamo, N. Russo, "A theoretical study of alkynes insertion into metal-hydride bond catalyzed by bimetallic complexes", *Inorg. Chem., ASAP*

[2] T. Le Bahers, **S. Di Tommaso**, C. Peltier, G. Fayet, R. Giacobazzi, V. Tognetti, A. Prestianni, F. Labat, "Acridine orange in a pumpkin-shaped macrocycle: Beyond solvent effects in the UV-visible spectra simulation of dyes", *J. Mol. Struct.: Theochem*, **2010**, 954, 45-51

[1] **S. Di Tommaso**, T. Marino, F. Rondinelli, N. Russo, M. Toscano, "CO₂ Activation by Nb⁺ and NbO⁺ in the Gas Phase. A Case of Two-State Reactivity Process", *J. Chem. Theory Comput.*, **2007**, 3, 811

✓ Publications dans des actes de congrès

S. Di Tommaso, P. Rotureau, A. Vignes, M. Alzerreca, W. Benaissa, C. Adamo, "Study of the peroxidation mechanism of diethyl ether (DEE)", SUTER G., DE RADEMAEKER E. (Eds.). Loss prevention and safety promotion in the process industries : proceedings of the 13th international symposium, 6-9 june 2010, Brugge, Belgium. Antwerpen : Technologisch Instituut, 2010, vol. 2, pp. 327-333.

✓ Communications

[3] 13th International Symposium on Loss Prevention and Safety Promotion in the Process Industry
06-09 juin 2010, Bruges (Belgique)

S. Di Tommaso, P. Rotureau, C. Adamo, "Study of the peroxidation mechanism of diethyl ether (DEE)" - COMMUNICATION ORALE

[2] 13th International Conference on the Applications of Density Functional Theory in Chemistry and Physics
31 août – 04 septembre 2009, Lyon (France)

S. Di Tommaso, P. Rotureau, C. Adamo, "Theoretical study of the peroxidation mechanism of diethyl ether" - POSTER

[1] XXXV Congresso Nazionale della Divisione di Chimica Inorganica della Società Chimica Italiana
03 - 07 settembre 2006, Milan (Italie)

S. Di Tommaso, T. Marino, F. Rondinelli, N. Russo, M. Toscano, "CO₂ activation by Nb⁺ and NbO⁺ in the gas phase. A case of two-state reactivity process" - POSTER