

PUBLICATIONS ET CONGRES (janvier 2014)

✓ Articles dans des journaux internationaux à comité de lecture

- [9] **S. Di Tommaso**, W. Benaissa, P. Grouez, P. Rotureau, C. Adamo, "A theoretical and experimental study on the inhibition of DEE oxidation", soumis (*Energy Fuel*)
- [8] **S. Di Tommaso**, H. David, J. Gomar, C. Adamo, "From iridoids to dyes: a theoretical study on genipin reactivity", accepté (*RSC Adv*).
- [7] **S. Di Tommaso**, P. Rotureau, B. Sirjean, R. Fournet, W. Benaissa, P. Gruez, C. Adamo, "A mechanistic and experimental study on the diethyl ether oxidation", *Process Saf. Prog.* DOI: 10.1002/prs.11621.
- [6] **S. Di Tommaso**, P. David, K. Picolet, M. Gabant, H. David, J.-L. Morançais, J. Gomar, F. Leroy, C. Adamo, "Structure of genipin in solution: a combined experimental and theoretical study", *RSC Adv.*, **2013**, 3, 13764-13771.
- [5] **S. Di Tommaso**, P. Rotureau, C. Adamo, "Oxidation mechanism of aliphatic ethers: theoretical insights on the main reaction channels", *J. Phys. Chem. A*, **2012**, 116, 9010-9019.
- [4] **S. Di Tommaso**, P. Rotureau, O. Crescenzi, C. Adamo, "Oxidation mechanism of diethyl ether: a complex process for a simple molecule", *Phys. Chem. Chem. Phys.*, **2011**, 13, 14636-14645.
- [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.*, **2010**, 49, 9875-9883.
- [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, 811-815.

✓ 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

- [10] XIV^{ème} Congrès de la Société Française de Génie des Procédés
08-10 octobre 2013, Lyon (France)
S. Di Tommaso, P. Rotureau, P. Gruez, W. Benaissa, C. Adamo, "Influence d'antioxydants dans le mécanisme d'oxydation de l'éther éthylique : étude théorique et expérimentale." - POSTER
- [9] European Materials Research Society 2013 Fall Meeting
16-20 septembre 2013, Varsovie (Pologne)
S. Di Tommaso, F. Labat, F. Giannici, A. Martorana, C. Adamo, "Structural and electronic properties of ion-exchangeable layered perovskite" - POSTER
- [8] MSSC2013, Ab initio Modelling in Solid State Chemistry 16-20 septembre 2013, Londres (UK)
S. Di Tommaso, F. Labat, F. Giannici, A. Martorana, C. Adamo, "Structural and electronic properties of ion-exchangeable layered perovskite" - POSTER

[7] 7th Molecular Quantum Mechanics Congress 02-07 juin 2013, Lugano (Suisse)
S. Di Tommaso, P. David, K. Picolet, M. Gabant, H. David, J.-L. Morançais, J. Gomar, F. Leroy, C. Adamo, "A combined experimental and theoretical study on the structure of genipin in solution" - POSTER

[6] 46th Loss Prevention Symposium part of the 8th Global Congress on Process Safety 01-04 avril 2012, Houston (TX - US)
S. Di Tommaso, P. Rotureau, W. Benaissa, P. Gruez, C. Adamo, "A mechanistic and experimental study of the diethyl ether oxidation" - COMMUNICATION ORALE

[5] XIII^{ème} Congrès de la Société Française de Génie des Procédés 29 novembre - 01 décembre 2011, Lille (France)
P. Rotureau, **S. Di Tommaso**, A. Vignes, W. Benaissa, C. Adamo, "Theoretical and experimental study of DEE autoxidation" - POSTER

[4] 7th International Conference on Chemical Kinetics 10-14 juillet 2011, Cambridge (MA - US)
S. Di Tommaso, P. Rotureau, B. Sirjean, P. A. Glaude, R. Fournet, F. Battin-Leclerc, C. Adamo, "A mechanistic and kinetical study of DEE oxidation" - POSTER

[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