

Liste des communications

Éric BRÉMOND

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1 Communications orales

1. Éric BRÉMOND. *Étude spectroscopique d'un fluorophore émettant de la lumière blanche : traitement par la DFT et la TD-DFT*. Journées de modélisation ENS-ENSCP, Paris, France, 19 mai 2011.
2. Éric BRÉMOND. *Prédiction ab initio de spectres UV-visibles*. Journée du LECIME, Paris, France, 5 avril 2011.
3. Éric BRÉMOND. *Ab initio Prediction of UV-visible Spectra*. Sanofi-Aventis Thesis Days, Arles, France, 1 octobre 2010.

2 Communications affichées

1. Éric BRÉMOND, Marta E. ALBERTO, Nino RUSSO, Carlo ADAMO. *Spectroscopic Study of An Organic White Light-Emitting Fluorophore : A DFT and TD-DFT Approach*. Excited states and non-adiabatic processes in complex systems. Theoretical approaches, Sant Feliu de Guíxols, Espagne, 25 au 27 juillet 2011.

3 Communications écrites

1. Éric BRÉMOND, Diane PILARD, Ilaria CIOFINI, Henry CHERMETTE, Carlo ADAMO, Pietro CORTONA. Generalized Gradient Exchange Functionals based on the Gradient-Regulated Connection : a New Member of the TCA Family. Submitted to *Theoretical Chemistry Accounts*.
2. Julien TOULOUSE, Kamal SHARKAS, Éric BRÉMOND, Carlo ADAMO. Rationale for a new class of double-hybrid approximations in density-functional theory. Submitted to *Journal of Chemical Physics*.
3. Éric BRÉMOND, Carlo ADAMO. Seeking for parameter-free double-hybrid functionals : The PBE0-DH model. *Journal of Chemical Physics*, 135(2) :024106, 2011.
4. Denis JACQUEMIN, Éric BRÉMOND, Aurélien PLANCHAT, Ilaria CIOFINI, Carlo ADAMO. TD-DFT vibronic couplings in anthraquinones : From basis set and functional benchmarks to applications for industrial dyes. *Journal of Chemical Theory and Computation*, 7(6) :1882–1892, 2011.

5. Éric BRÉMOND, Jérôme KIEFFER, Carlo ADAMO. A reliable method for fitting TD-DFT transitions to experimental UV-visible spectra. *Journal of Molecular Structure : THEOCHEM*, 954(1-3) :52-56, 2010.
6. Jérôme KIEFFER, Éric BRÉMOND, Philippe LIENARD, Giovanni BOCCARDI. In silico assessment of drug substances chemical stability. *Journal of Molecular Structure : THEOCHEM*, 954(1-3) :75-79, 2010.
7. Paul L. A. POPELIER, Éric BRÉMOND. Geometrically faithful homeomorphisms between the electron density and the bare nuclear potential. *International Journal of Quantum Chemistry*, 109(11) :2542-2553, 2009.