

# SURFACE EFFECTS IN ENANTIOSELECTIVE COPPER (I) CATALYSIS

Gonzalo Jiménez-Osés,<sup>1,\*</sup> José I. García<sup>2</sup>, José A. Mayoral<sup>2</sup>

<sup>1</sup>Departamento de Química, Universidad de La Rioja, Centro de Investigación en Síntesis Química, E-26006 Logroño, Spain.

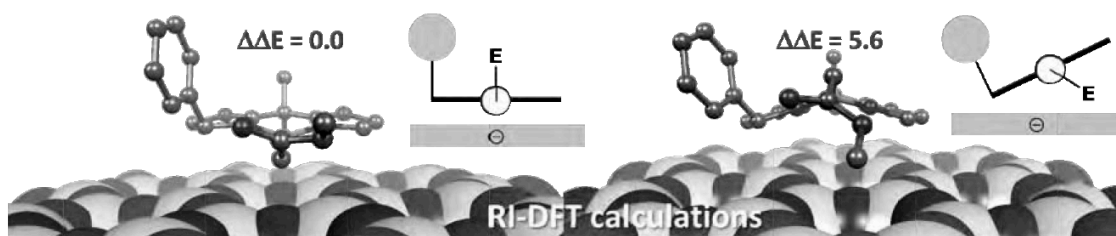
<sup>2</sup>Instituto de Síntesis Química y Catálisis Homogénea (ISQCH) and Department of Organic Chemistry, Facultad de Ciencias.

CSIC-Universidad de Zaragoza, C/Pedro Cerbuna, 12, E-50009 Zaragoza, Spain

e-mail: gonzalo.jimenez@unirioja.es

Chiral bisoxazoline-copper complexes are efficient enantioselective catalysts for many organic transformations. When these cationic complexes are immobilized onto clays through electrostatic interactions, strong support confinement effects have been observed, able to completely change the stereoselectivity of several reactions, and in particular of that of styrene cyclopropanation with diazoesters. Ligand design allows improving confinement effects in the case of *cis/trans* stereoselectivity.<sup>[1]</sup>

In an effort to rationalized these results, we have accomplished a computational study in which the relative energies of the key reaction intermediates, supported on a model clay through ionic pair interactions, have been evaluated using DFT methods.<sup>[2]</sup>



- 1) Fernández, A. I.; Fraile, J. M.; García, J. I.; Herrerías, C. I.; Mayoral, J. A.; Salvatella, L. *Catal. Commun.* **2001**, *2*, 165; Fraile, J. M.; García, J. I.; Herrerías, C. I.; Mayoral, J. A.; Pires, E. *Chem. Soc. Rev.* **2009**, *38*, 695.
- 2) a) Fraile, J. M.; García, J. I.; Martínez-Merino, V.; Mayoral, J. A.; Salvatella, L. *J. Am. Chem. Soc.* **2001**, *123*, 7616; b) García, J. I.; Jiménez-Osés, G.; Martínez-Merino, V.; Mayoral, J. A.; Pires, E.; Villalba, I.; *Chem. Eur. J.* **2007**, *13*, 4064; c) García, J. I.; Jiménez-Osés, G.; Mayoral, J. A.; *Chem. Eur. J.* **2011**, *17*, 529.