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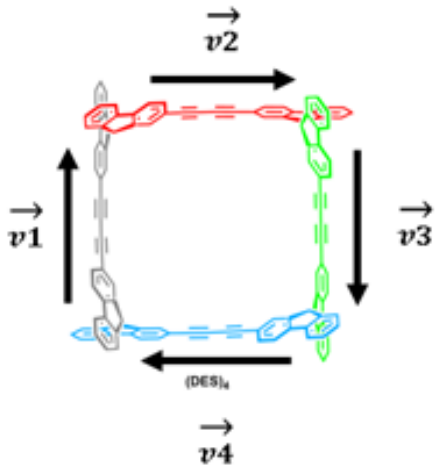
Understanding Chirality for the Design of Tailored Chiroptical Systems

S. Castro-Fernández, M. M. Cid, C. S. López, A. Navarro-Vázquez, R. Mosquera, J.L. Alonso-Gómez

University of Vigo
silvia@uvigo.es

Finding new model structures with high recognition capability and intense chiroptical responses has been recently an intense area of research. The promising results obtained during the last years on the alleno-acetylenic synthesis prompted the development of different chiral structures looking for the improvement of the chiroptical responses–shape-persistency relationship.[1–3] However, photoisomerization of diethynylallenes (**DEAs**) when attached to electron-donating substituents limits the functionalization of chiral macrocycles. Our recent theoretical and experimental studies support the replacement of **DEAs** by diethynylspiranes (**DESs**) as more stable chiral building blocks.[4]



In order to facilitate the development of chiroptical applications, the multiple exciton coupling method has been developed. This tool allows the rapid geometry/chiroptical-response analysis of systems bearing several identical chromophores for the design of potent chiroptical systems.

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[2] S. Míguez-Lago, A. L. Llamas-Saiz, M. Magdalena Cid, J. L. Alonso-Gómez, *Chem. Eur. J.* **2015**, DOI 10.1002/chem.201503994.

[3] S. Castro-Fernández, I. R. Lahoz, A. L. Llamas-Saiz, J. L. Alonso-Gómez, M.-M. Cid, A. Navarro-Vázquez, *Org. Lett.* **2014**, *16*, 1136–1139.

[4] S. Castro-Fernández, M. M. Cid, C. S. López, J. L. Alonso-Gómez, *J. Phys. Chem. A* **2015**, *119*, 1747–1753.