The mechanism of the two-step spin-transition of a thiazyl-diradical-based material presenting geometrical frustration.

Researchers:
Juan Jose Novoa Vide. Facultat de Química. Universitat de Barcelona.

Idioma Indefinido

Descrição:
Proyecto asignado a través de la Red Española de Supercomputación [1].

Recent years have witnessed a growing interest in the research of molecular materials that can be switched between two different states through the application of an external stimulus (e.g. heat, light) because these materials have a great potential for application in sensors, displays and in information technology. The main goal of this Activity is to understand the mechanisms underlying the two-step spin transition of a recently-prepared material made of bis-dithiadiazolyl diradicals and to decipher the origin of the geometrical frustration of one of its phases. Our results will provide useful insights on how to properly harness labile pi-pi interactions in stacks of diradicals in order to develop new diradical-based switchable materials.

Ligações
[1] https://www.res.es/