



Showcasing research from Professor Maseras laboratory, Institute of Chemical Research of Catalonia (ICIQ-CERCA), Catalonia, Spain.

Straightforward computational determination of energy-transfer kinetics through the application of the Marcus theory

Density functional theory is shown to be a reliable tool to estimate energy-transfer Gibbs energy barriers between different photosensitizers and organic molecules containing and alkene group.

### As featured in:



See Albert Solé-Daura and Feliu Maseras, *Chem. Sci.*, 2024, 15, 13650.