



Showcasing research conducted at the European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*, Trento, Italy) with the collaboration of the Universities of Murcia and Alacant (Spain).

Electronic excitation spectra of cerium oxides: from *ab initio* dielectric response functions to Monte Carlo electron transport simulations

Ab initio-informed Monte Carlo electron transport simulations are carried out in cerium oxides, which are materials relevant for applications ranging from catalysis to radiotherapy sensitisation. The energy- and momentum-dependent dielectric properties of these solids, obtained from high-accuracy first principles calculations, allow accurate interpretation of their measured REEL spectra lineshapes, yielding fairly good agreement.

As featured in:



See Simone Taioli, Maurizio Dapor *et al.*, *Phys. Chem. Chem. Phys.*, 2021, **23**, 19173.