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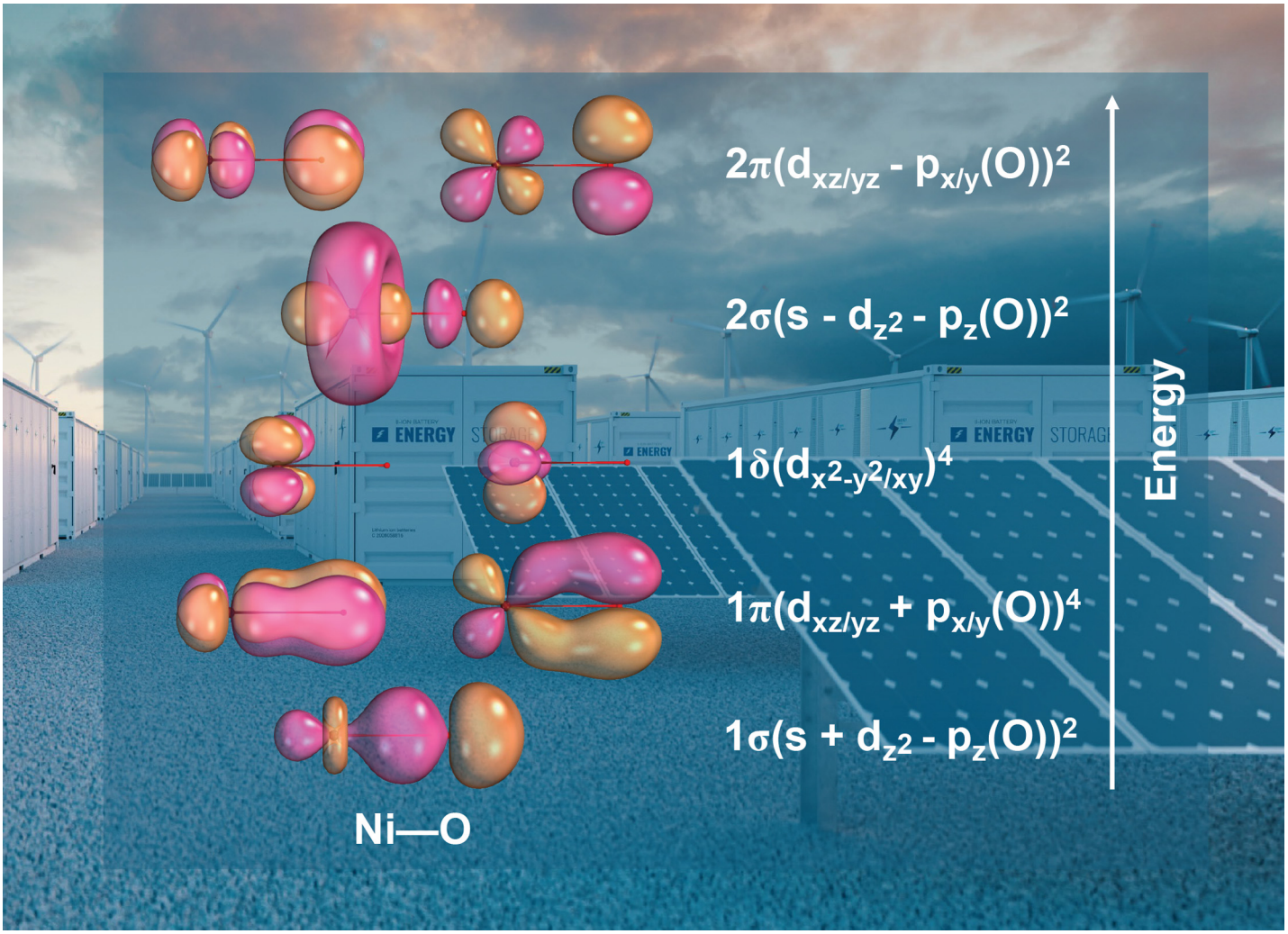

Showcasing research from Professor David Dixon's laboratory, Department of Chemistry & Biochemistry, The University of Alabama, USA.

The electronic structure of diatomic nickel oxide

The electronic structure of diatomic NiO using CASSCF, icMRCI+Q, CCSD(T), and DFT was predicted. There is significant ionic character with the $2p_z$ of O forming a σ bond with the $4s/3d_{z2}$ of the Ni. It is difficult to calculate the vibrational frequency but icMRCI+Q provides a reliable value. The calculated FPD bond dissociation energy is in good agreement with the lower experimental value. 43 DFT functionals were benchmarked to provide guidance for describing more complex NiO systems with only 3 functionals predicting the frequency correctly.

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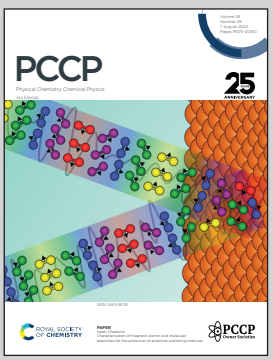

See David A. Dixon *et al.*, *Phys. Chem. Chem. Phys.*, 2024, **26**, 19646.

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