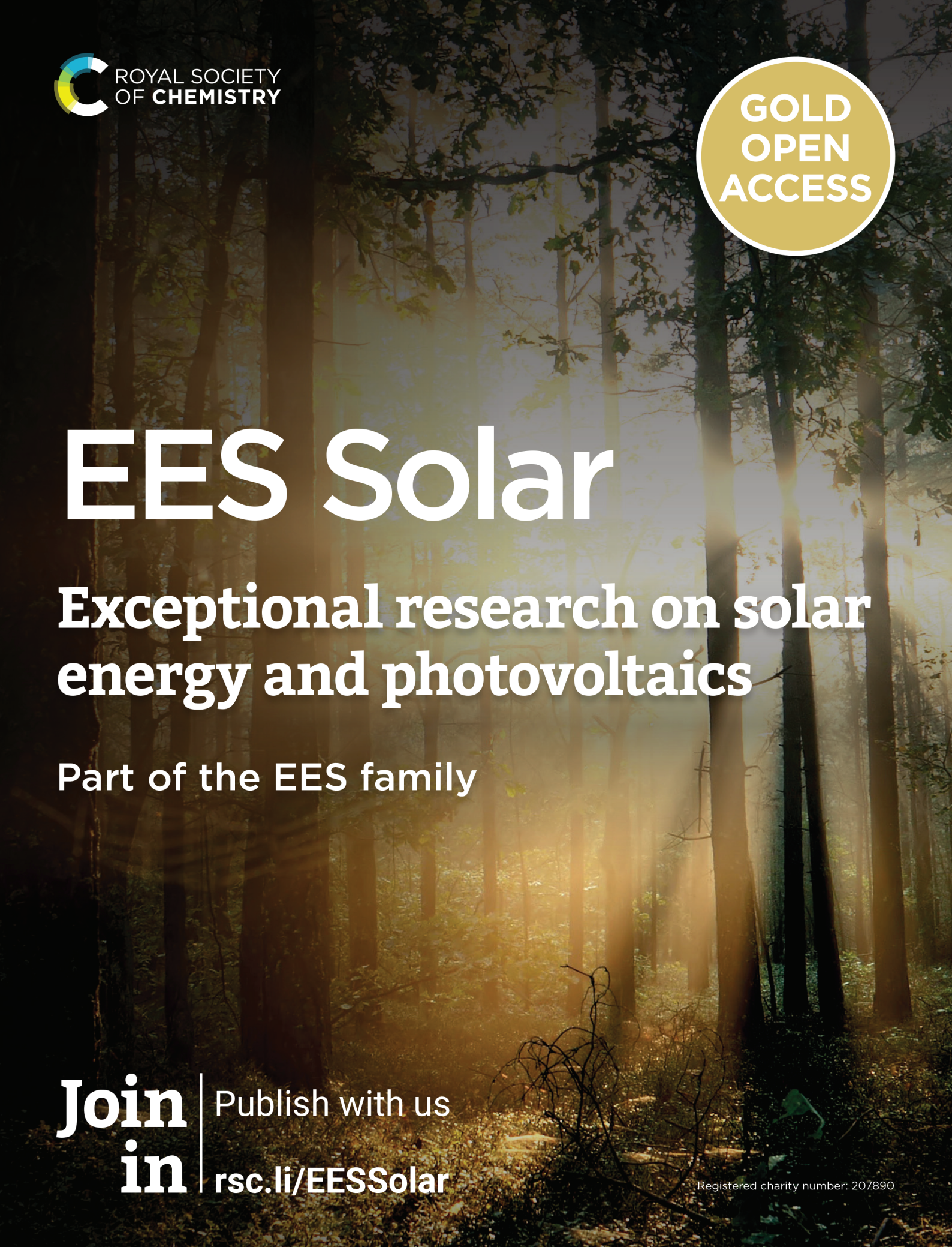
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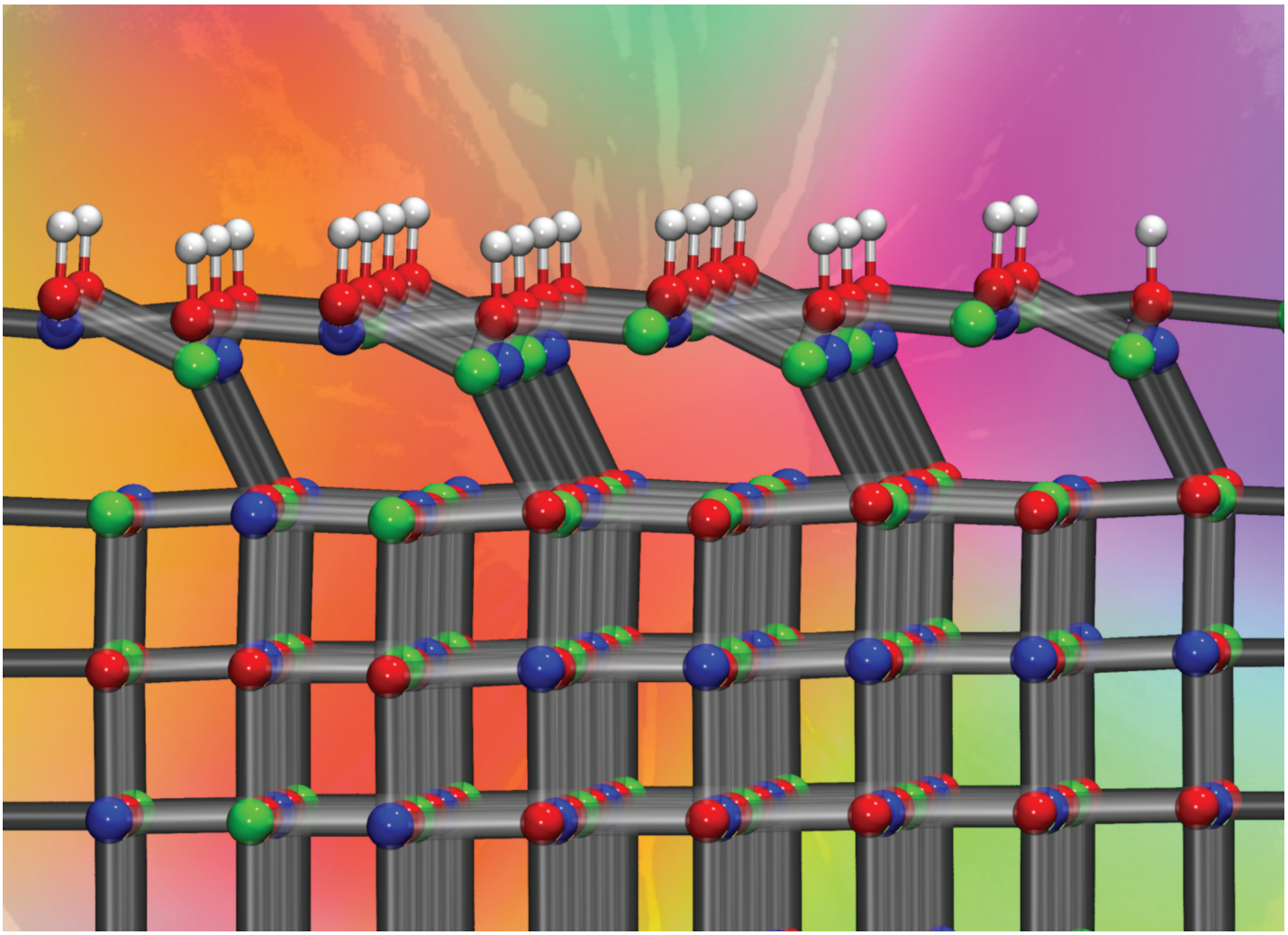

**Showcasing research from Insubria University – Department of Science and High Technology, and INSTM, Como, Italy, and Padova University - Department of Chemical Sciences, CNR-ICMATE and INSTM, Padova, Italy.**

Impact of –OH surface defects on the electronic and structural properties of nickel oxide thin films

Hydroxyl defects on NiO(100) surfaces significantly affect both the structure and the electronic properties of nickel-oxide nanomaterials. Density Functional Theory modeling shows that the defect chemical nature and their concentration directly influence the material electronic properties. This insight offers the opportunity of fine-tuning the electronic gap, or even switching from p-type to n-type character. At high coverages, the presence of –OH defects induces a significant reconstruction of the (100) surface, leading to the formation of under-coordinated Ni sites. This feature might enhance the system surface reactivity in relevant catalytic processes involving the target NiO-based materials.

## As featured in:


See Davide Barreca, Gloria Tabacchi *et al.*, *Dalton Trans.*, 2025, **54**, 2765.

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