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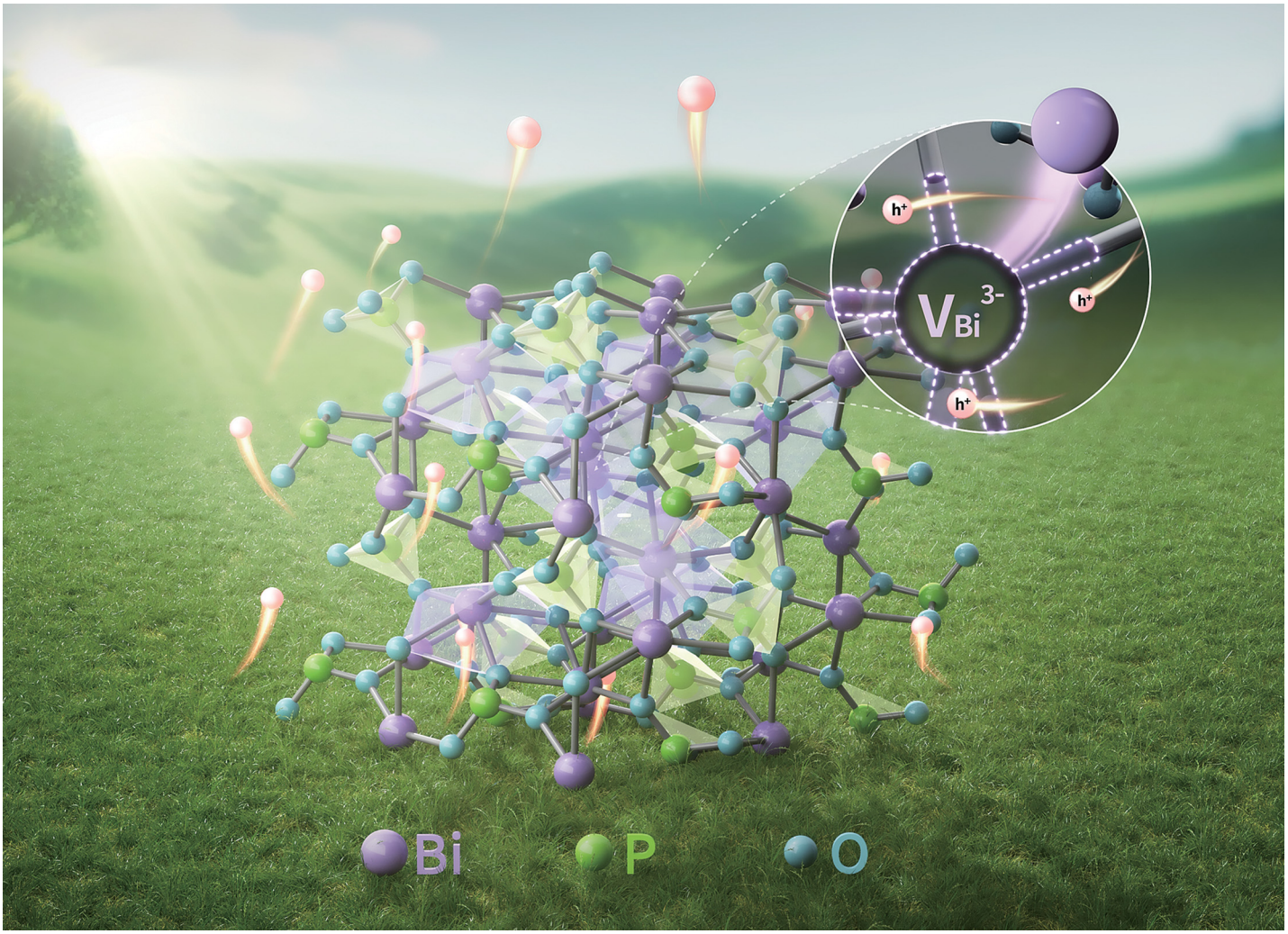

Showcasing research from the School of Physics and Astronomy, China West Normal University, Nanchong, China

Defect physics of intrinsic point defects in $BiPO_4$ photocatalysts: a hybrid functional study

It is well known that defects are inevitable in the process of preparing crystals in experiments, and they could significantly affect the properties of materials. In this work, *via* first principle calculations, we find that high hole carrier concentration can be achieved under O-rich, extreme Bi-poor, and certain high-temperature growth conditions in $BiPO_4$. The Bi vacancy in the –3 charge state is the major origin for this significant character.

As featured in:

See Bo Kong, Wentao Wang *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 30848.

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