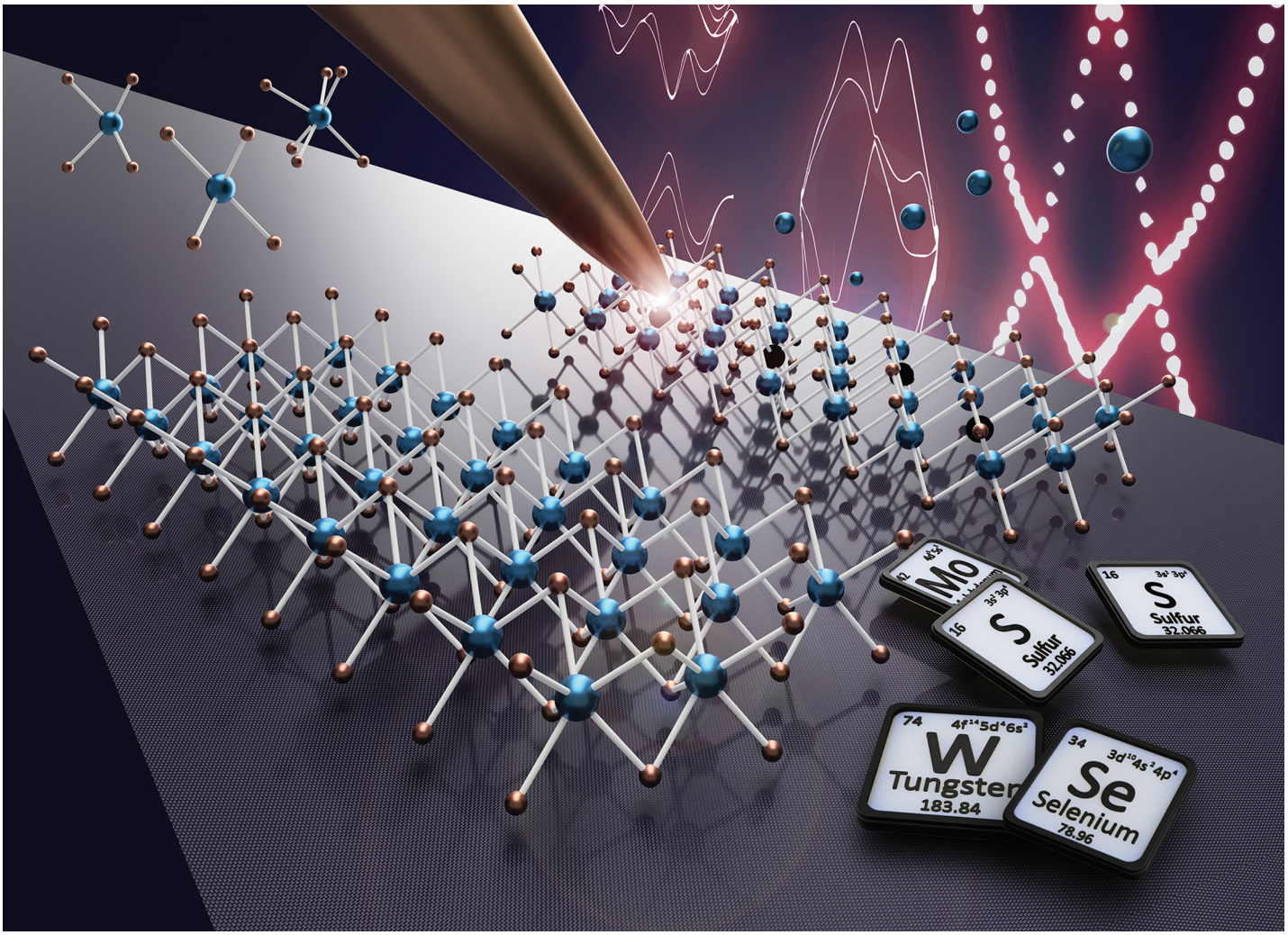

Showcasing research from Assoc. Prof. Berna Akgenç Hanedar and Assoc. Prof. Mehmet Cengiz Onbaşlı at Koç University, Türkiye.

Defect dependent electronic properties of two-dimensional transition metal dichalcogenides (2H, 1T, and 1T′ phases)

This study investigates the 2H, 1T, and 1T′ phases of MoS_2, WS_2, $MoSe_2$, and WSe_2, focusing on the influence of vacancy defect densities (3.13% to 21.88%) on their electronic band structures through density functional theory (DFT). Creating vacancies leads to the formation of defect bands that lead to a significant reduction in band gap energy, and this tunability highlights the potential for applications in quantum technologies and photonic devices.

As featured in:

See Berna Akgenc Hanedar and Mehmet Cengiz Onbaşlı, *Phys. Chem. Chem. Phys.*, 2025, **27**, 1809.

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