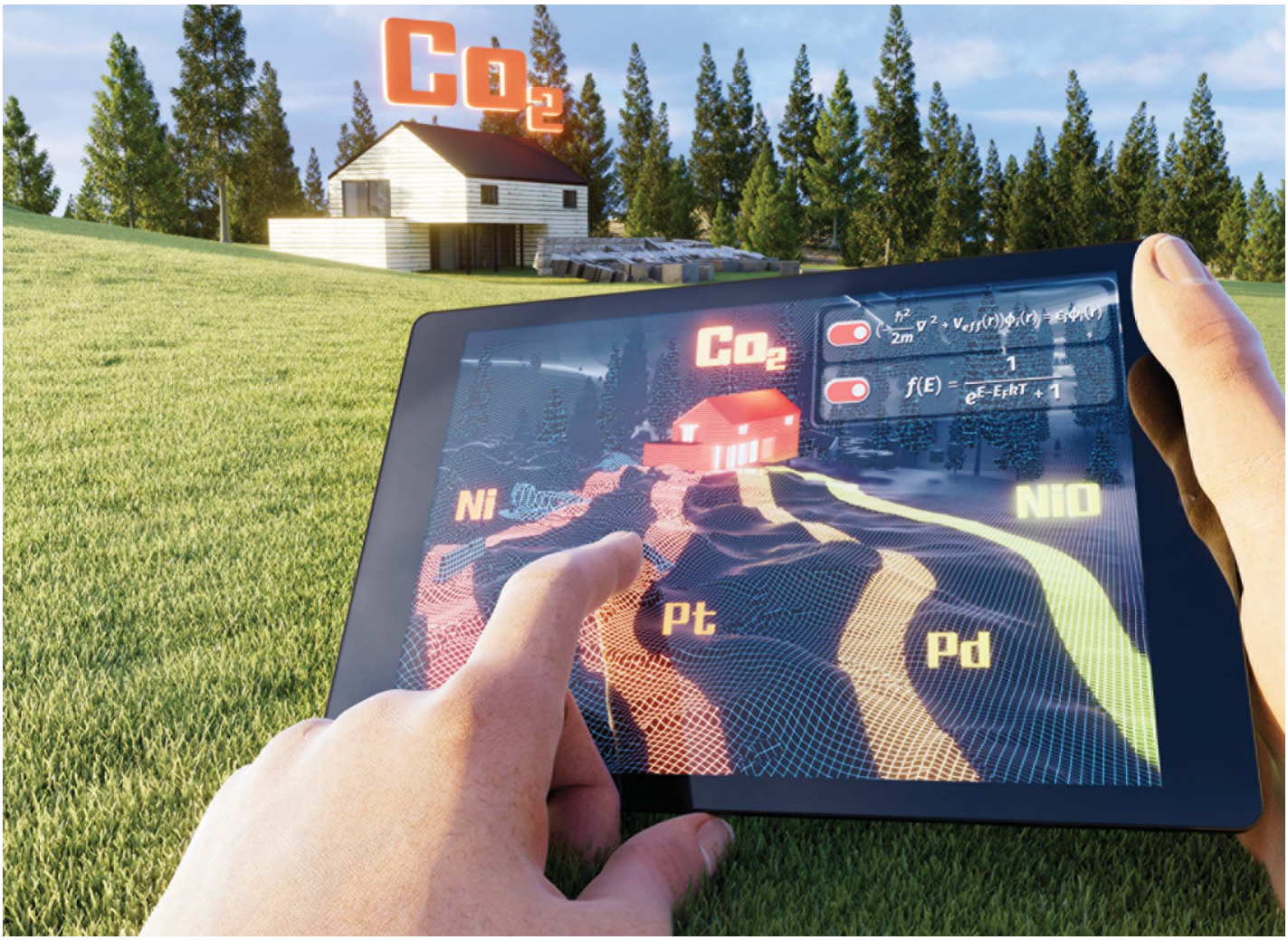

Showcasing research from laboratories of Professor Choi, School of Science, Xi'an Jiaotong-Liverpool University, Suzhou, China, Professor Cho, Department of Materials Science & Engineering, Ajou University, Suwon, Korea, and Dr. Ko, Korea Institute of Ceramic Technology, Jinju, Korea.

Overcoming the limitations of atomic-scale simulations on semiconductor catalysis with changing Fermi level and surface treatment

A new method of density functional theory calculation introduced in this article allows accurate predictions of surface reactions on wide band gap semiconductors in atomic-scale without limitations of cell size, which was not possible with conventional density functional theory calculations.

As featured in:

See Hyunseok Ko, Sung Beom Cho, Heechae Choi *et al.*, *J. Mater. Chem. A*, 2024, **12**, 33537.

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