

**Showcasing research from Professor Sato's laboratory, Kyoto University and Professor Onishi, Kobe University, Japan.**

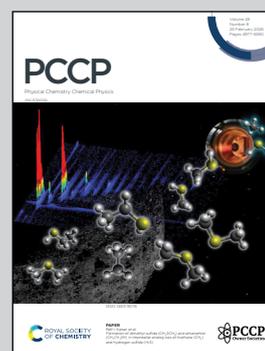
Dopant distributions and band-edge positions in Sr-doped  $\text{NaTaO}_3$ : a first-principles study

In this work, we performed first-principles calculations on an archetypal photocatalyst, Sr-doped  $\text{NaTaO}_3$ , to connect dopant distributions with band-edge modulation. We show that short Sr-Sr separations are thermodynamically favoured, explaining the experimentally suggested near-surface Sr enrichment. Sr-rich layers form in-gap states and shift both valence- and conduction-band edges upward, creating a built-in electric field that promotes charge separation and suppresses recombination. These findings highlight dopant-distribution engineering as a design principle beyond gap narrowing.

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See Hiroki Uratani *et al.*,  
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