

Unraveling Atomic Ordering and Epitaxial Strain Effects in Pd-Templated Pt–Cu Alloys for Hydrogen Oxidation

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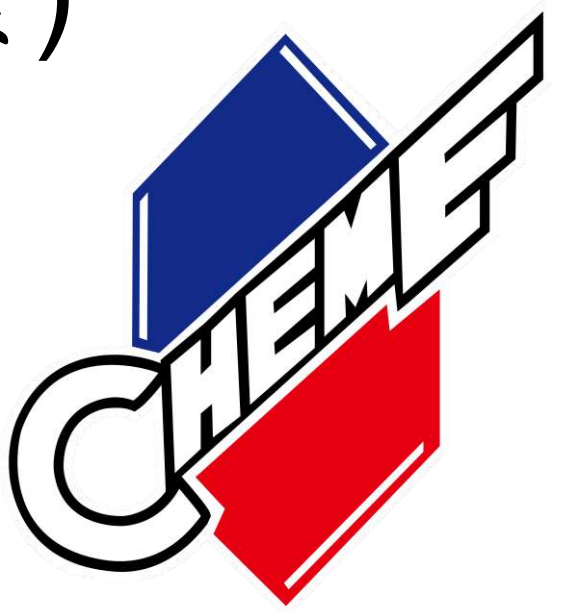


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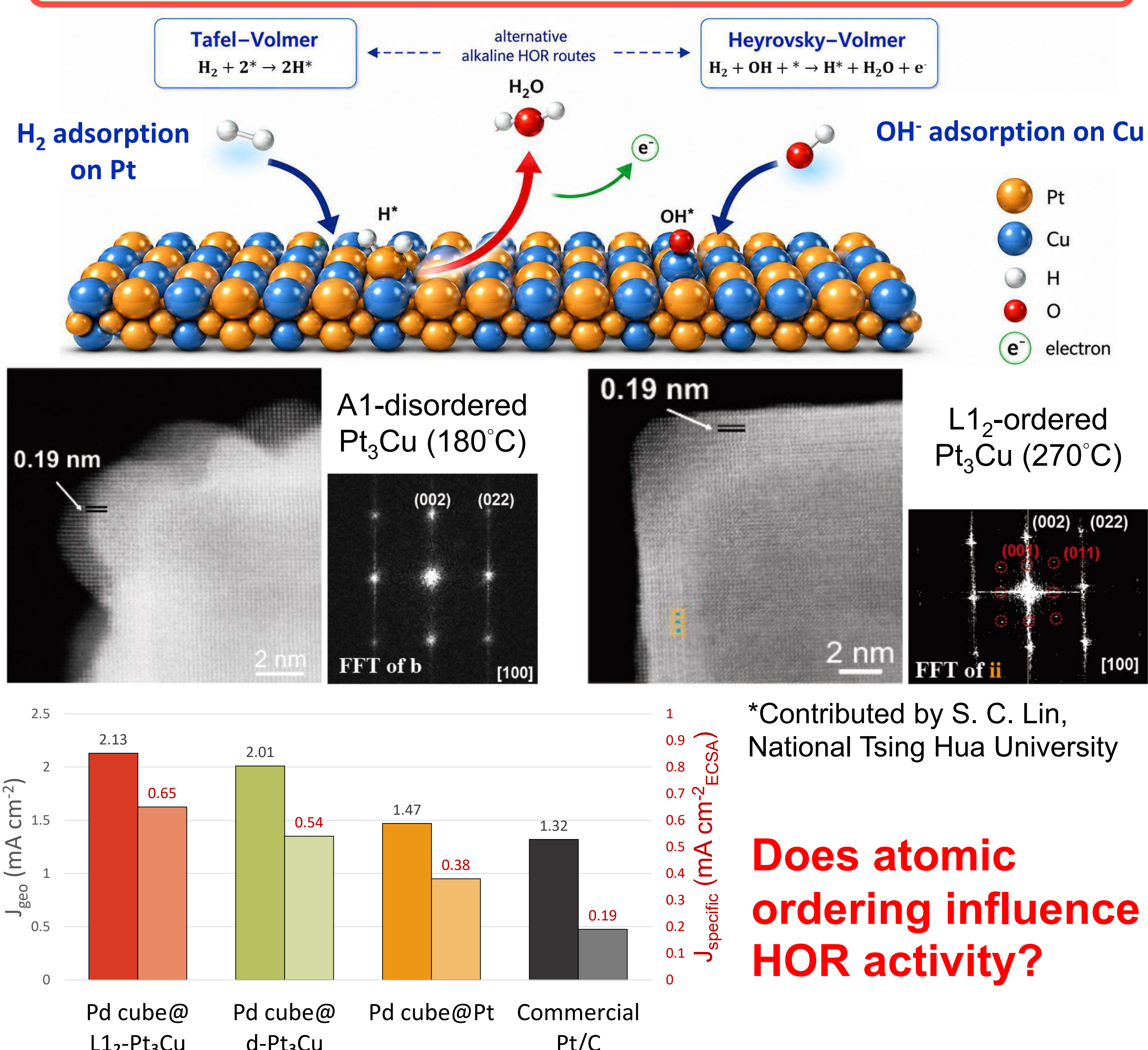


Introduction

Anion-exchange membrane fuel cells are limited by the sluggish kinetics of the hydrogen oxidation reaction (HOR) under alkaline conditions. HOR activity has been correlated with surface electron-accepting tendency and H₂/OH adsorption strengths.^[1] In bimetallic catalysts, these properties may be further influenced by atomic ordering and epitaxial strain. In Pd-cube-templated Pt–Cu synthesis, A1-type disordered Pt₃Cu was observed at 180°C, whereas ordered L1₂-Pt₃Cu formed at 270°C. This raises a fundamental question: how do atomic ordering and Pd-induced epitaxial constraints modify Pt–Cu properties? Here, DFT is used to evaluate Pt–Cu structural stability and lattice matching with Pd and to construct Pd-constrained surface models for subsequent electronic and HOR-relevant adsorption analyses.

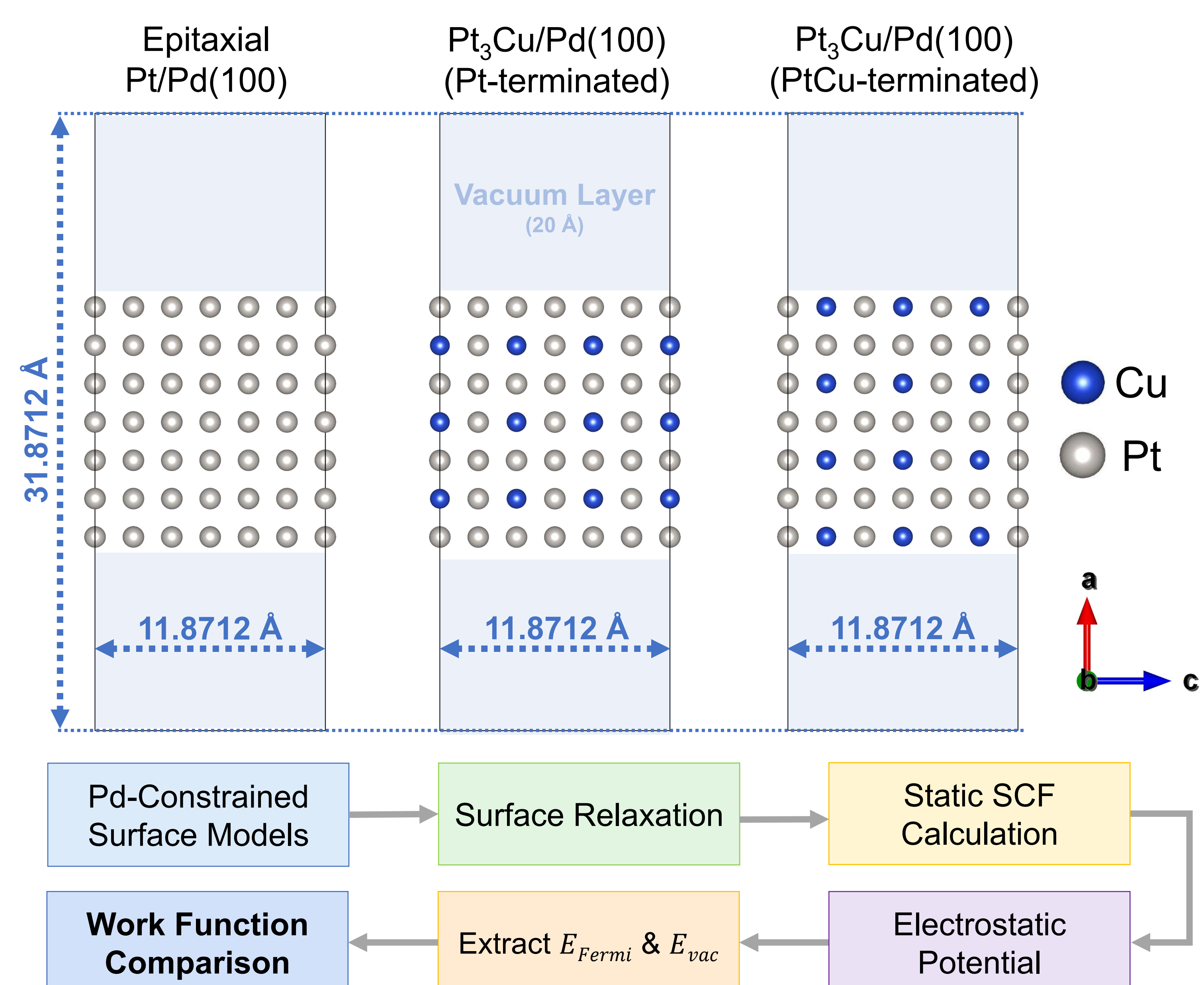
How do atomic ordering and Pd-induced epitaxial constraints modify the structural and electronic properties of Pt–Cu alloys?

HOR Mechanism & Experimental Motivation



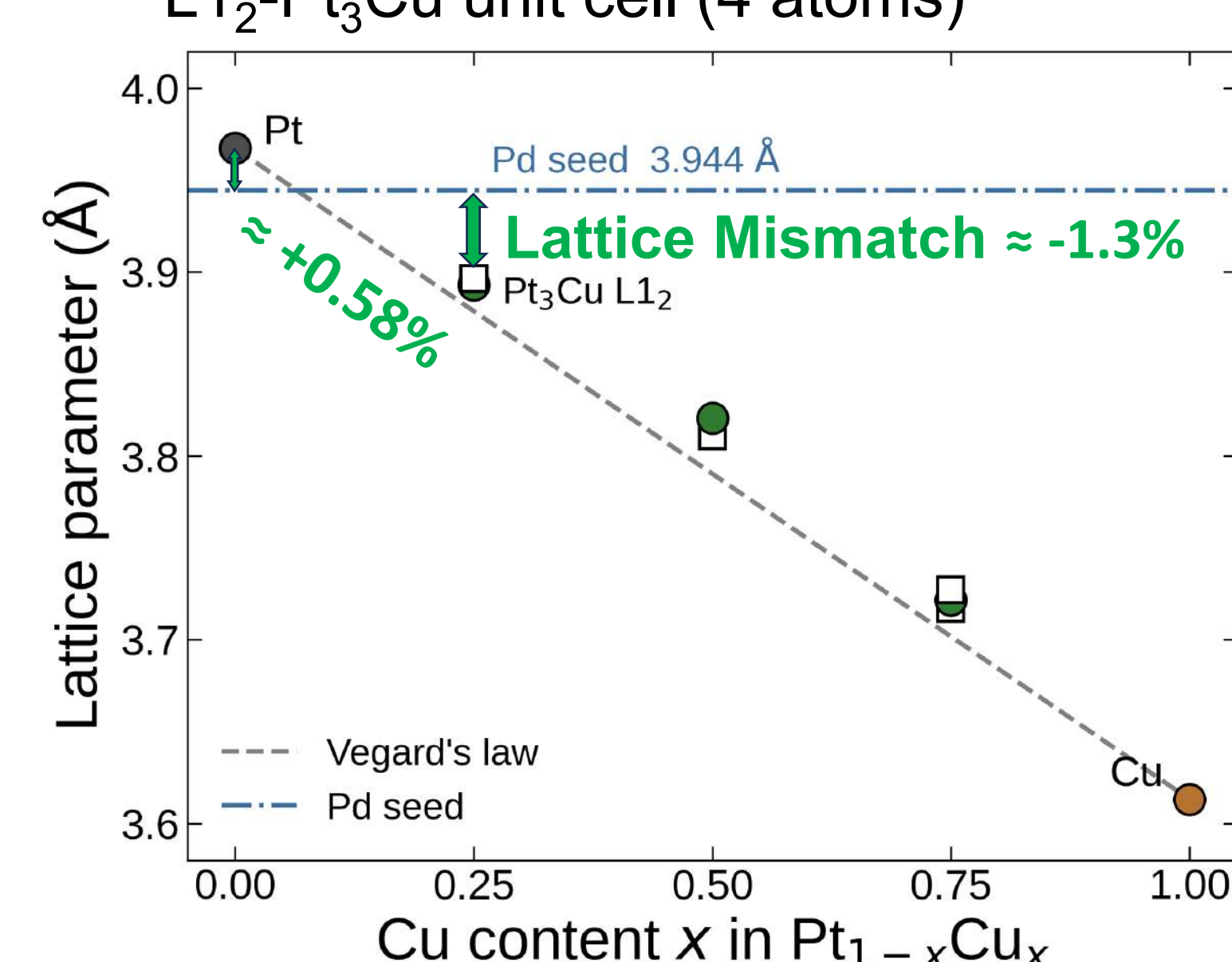
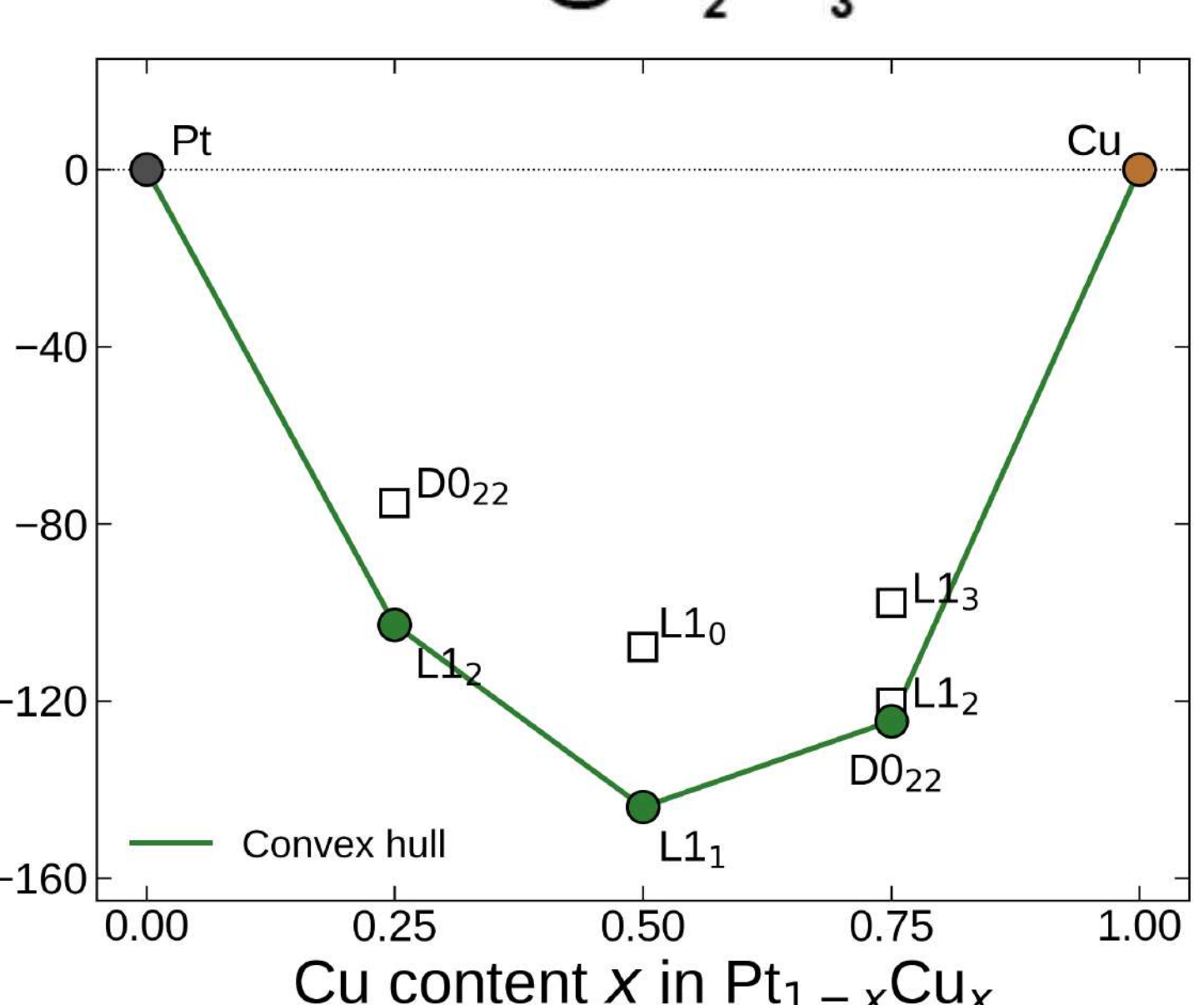
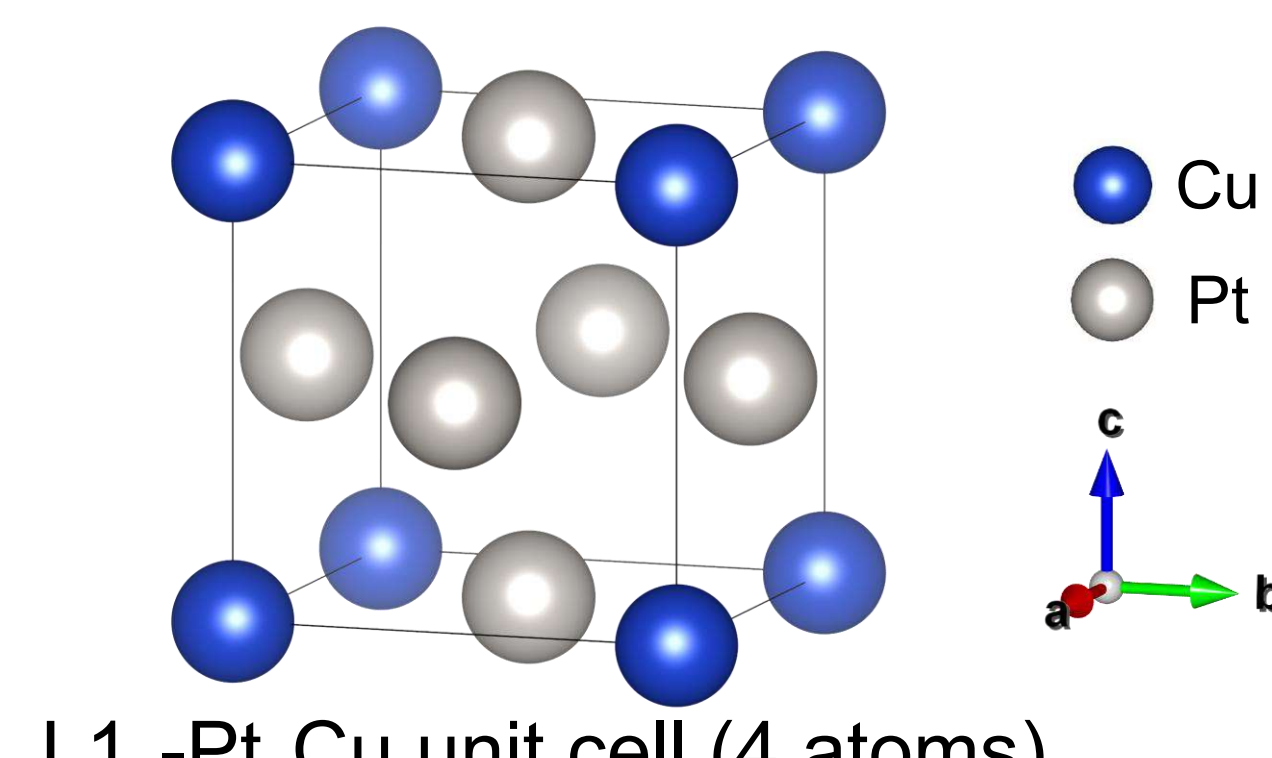
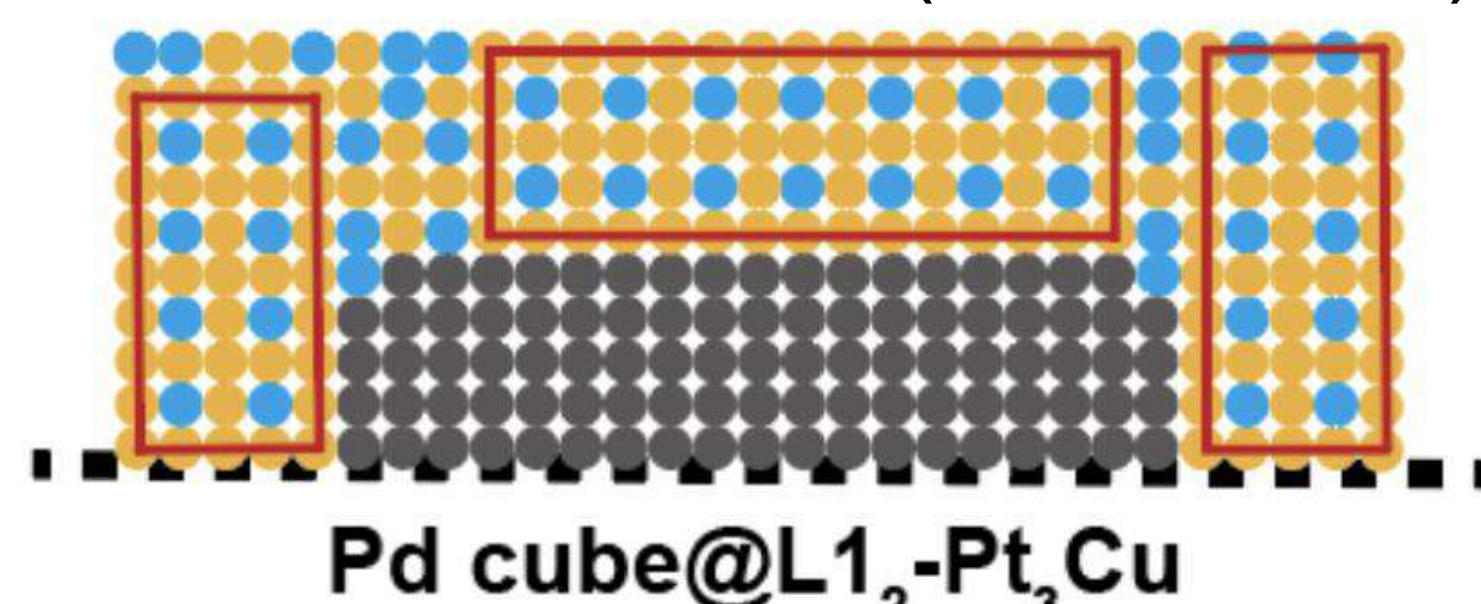
Does atomic ordering influence HOR activity?

Pd-Templated Surface Modeling & Computational Workflow



Atomic Ordering & Bulk Modeling

270°C, Pt-rich feed (Pt:Cu = 3: 1)



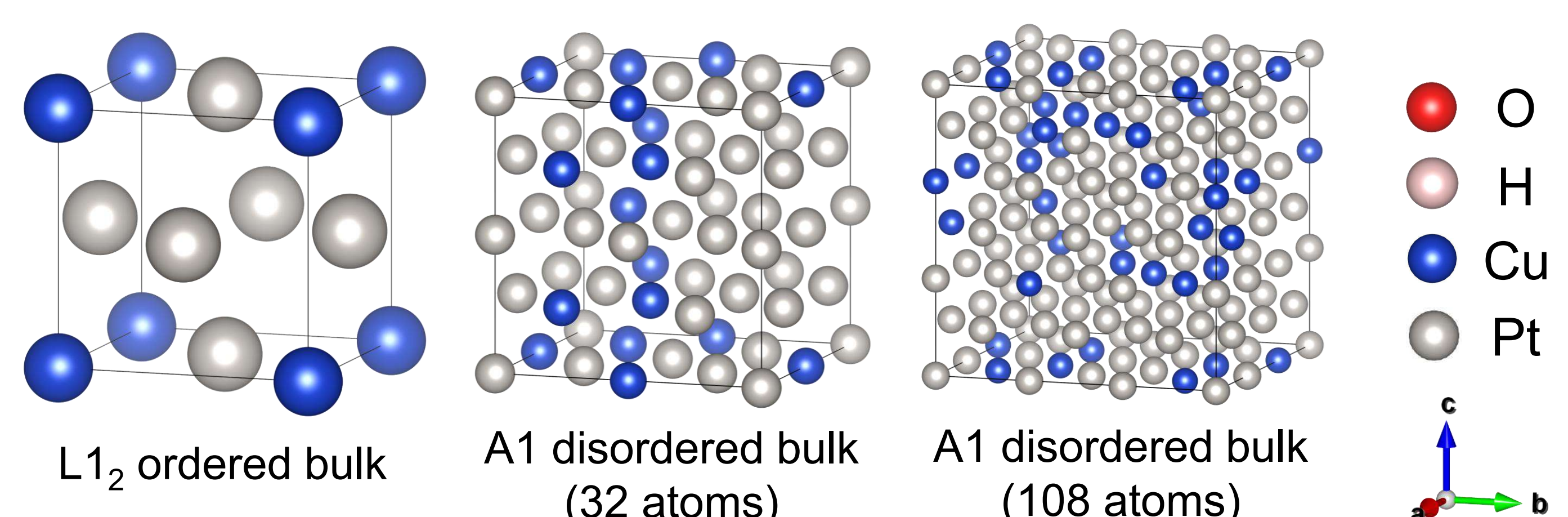
Pt-rich ordered Pt–Cu phases show smaller lattice mismatch with the Pd template.

References

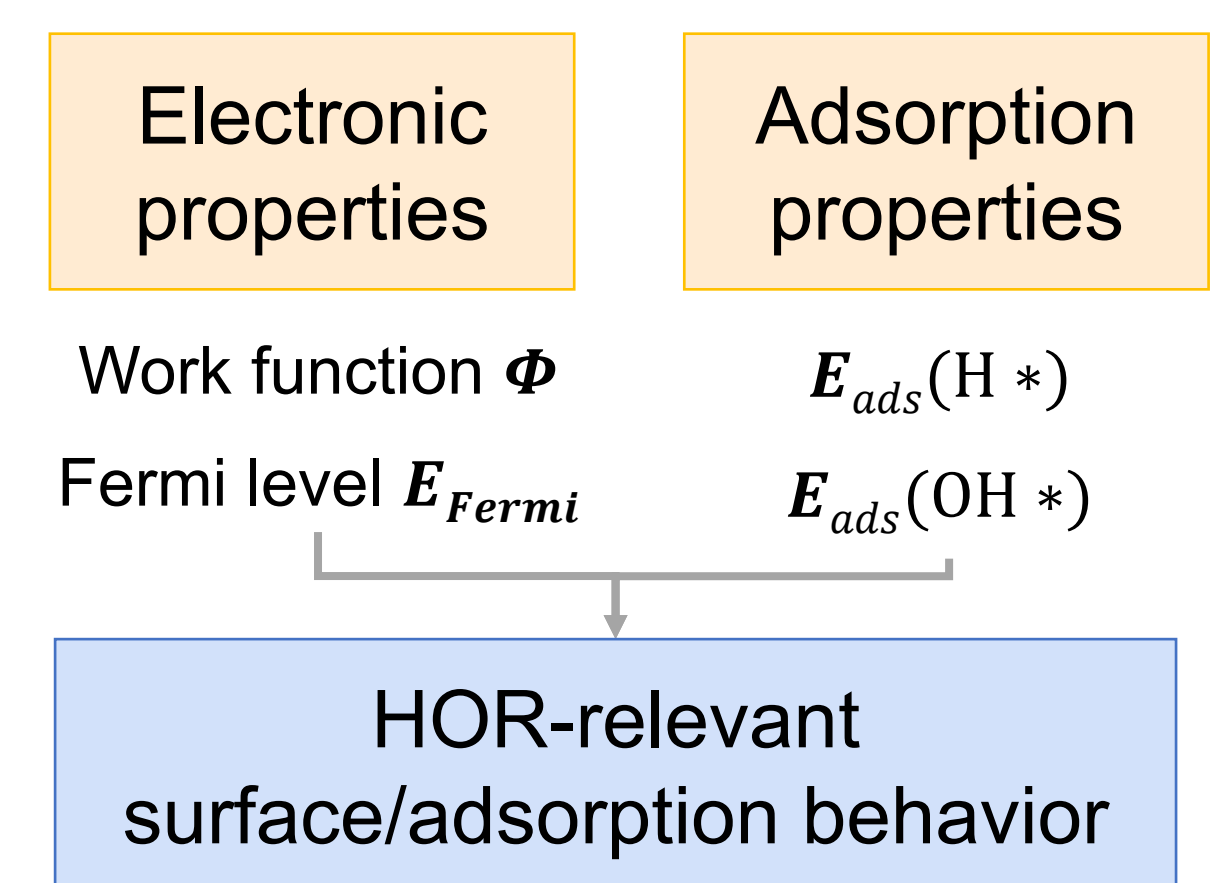
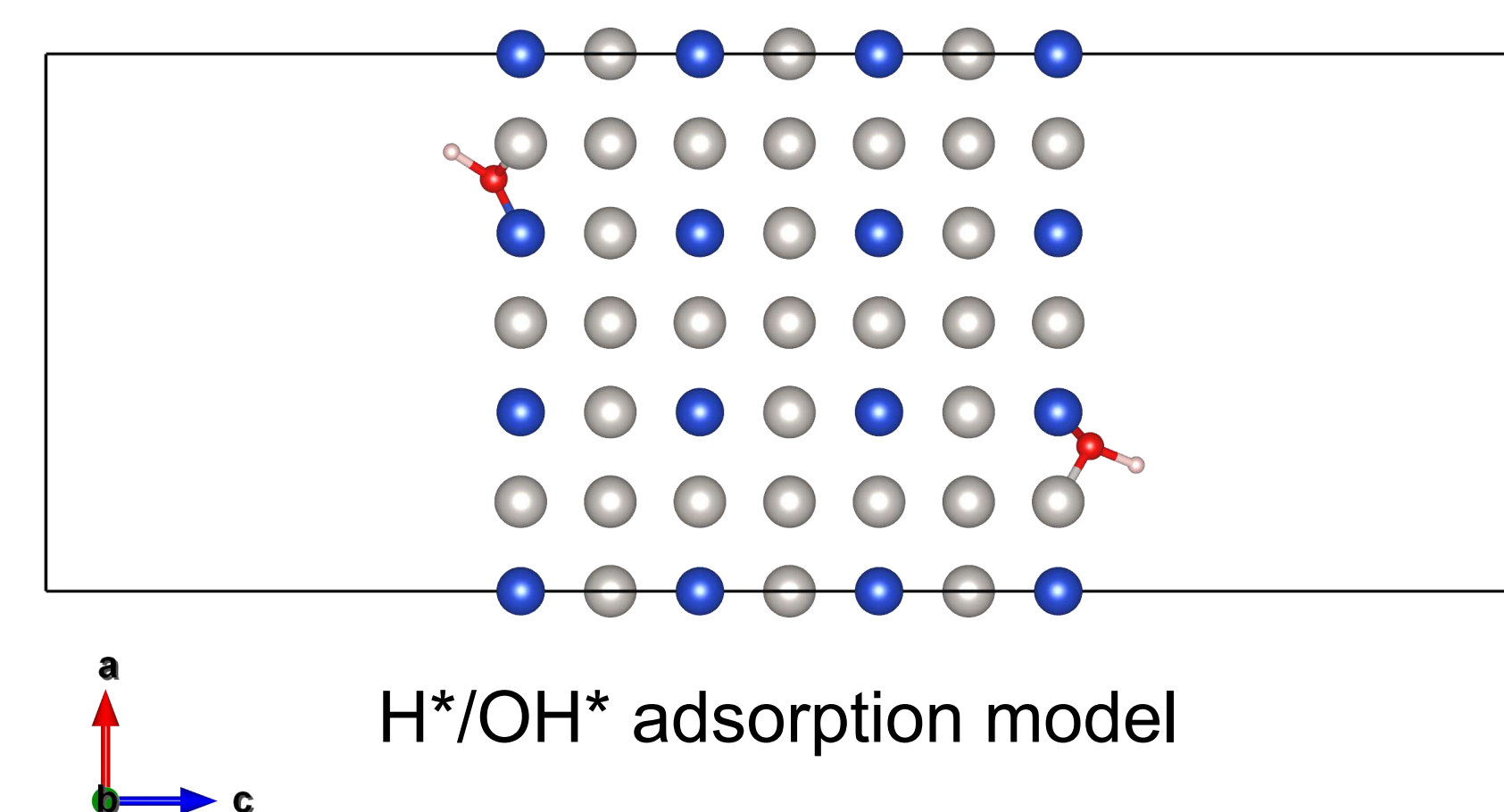
[1] Kao, IT., Kuo, RT., Lin, SC. et al. Exploring a bimetallic catalyst family for hydrogen oxidation with insights into superior activity and durability. Nat Commun 16, 10504 (2025).

Future Work

Model the Experimentally Observed A1-Disordered Pt₃Cu



Apply identical Pd-imposed constraints and construct surface models



Relate atomic ordering and Pd-induced strain to HOR-relevant properties