

Supplementary Materials:

Preferential Segregation of Gold at Symmetrical Tilt Grain Boundaries of Platinum: An Atomic-Scale Quantitative Understanding

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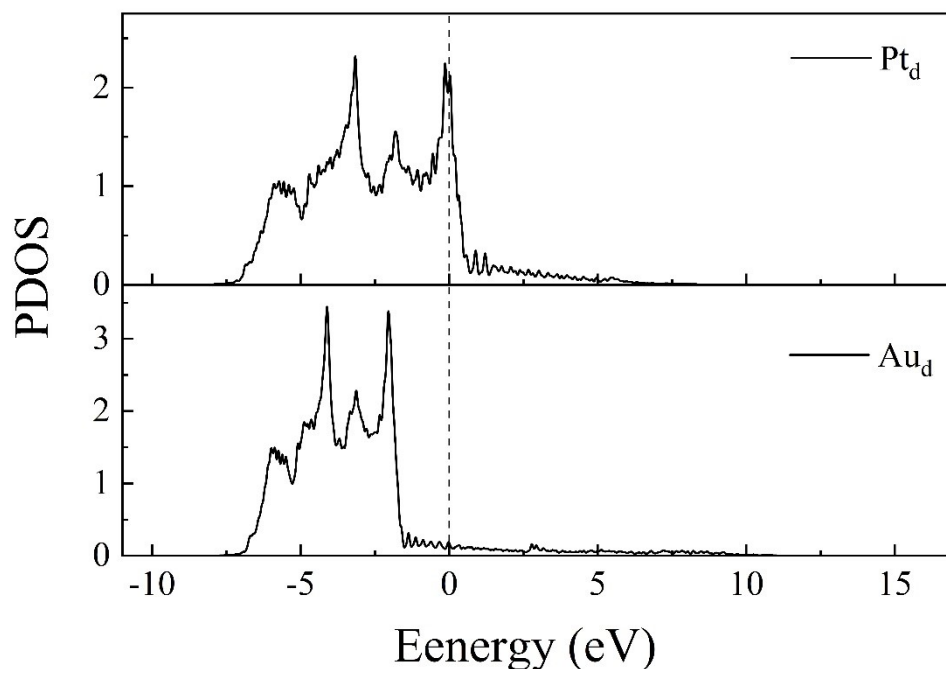


Fig. S1 PDOS diagram of d-band for Pt and Au.

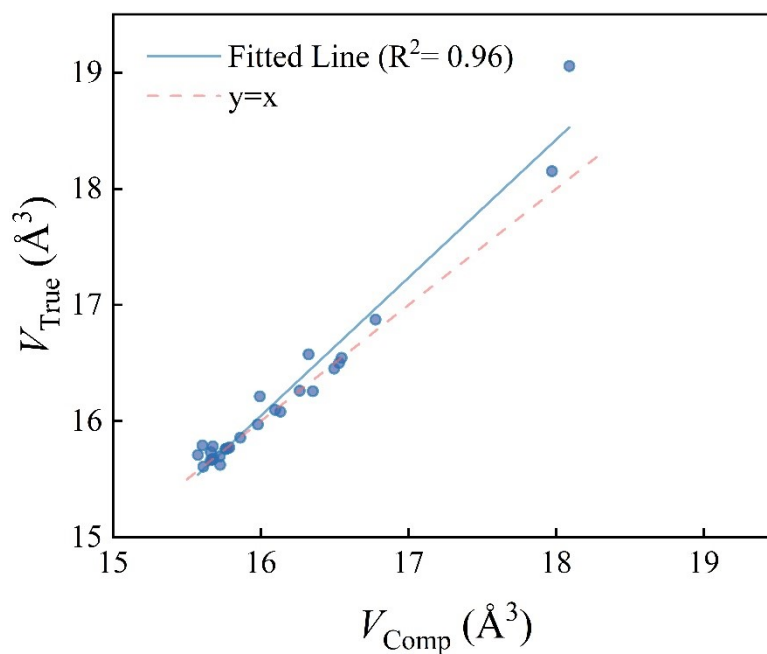


Fig. S2 Comparison between the true atom Voronoi volume and compute values based on Eq. 8.

Utilizing the average bond length rather than specific bond length for volume calculation results in

$V_{\text{Comp}} < V_{\text{True}}$, with a slope exceeding 1.