Calculated atomic arrangement and impurity bonding at a \( \kappa \)-Alumina – Al(771) interface.\(^1\) PETER J. FEIBELMAN, Sandia National Laboratories — First principles optimization of a \( \kappa \)-Alumina – Al(771) superlattice shows that the incompressible oxide causes substantial disorder in the adjacent, soft metal layers. An H “probe atom” is found to bind best in the disrupted metal region, suggesting that this is the locus of initial failure of a protective oxide layer.

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