Age old antipodes united: stable and low-work-function surfaces are generic

M.A. UIJTTEWAAL, G.A. DE WIJS, R.A. DE GROOT, Radboud University Nijmegen/Electronic Structure of Materials — Both a low work function and a stable surface are crucial for the application of cathodes in e.g. microwave ovens, organic photoconductors and displays as CRTs and OLEDs. Until recently they were considered antipodes. In previous work[1] we showed a stable low-work-function surface to be realised for the compound BaAl$_4$ and even predicted that stable, low-work-function surfaces would be generic for metals with polar surfaces. Now, \textit{ab initio} calculations confirm the prediction for the compounds CaAl$_4$, BaAuIn$_3$ and LaB$_6$.