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Computing properties of Pt surfaces for understanding electron emission

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Electron emission from a surface, and ultimately electrical breakdown, will be governed by local heterogeneity in composition, structure and work function across a substrate. Even for a seemingly simple substrate such as Platinum, without contaminants or adsorbed layers, understanding of the surface structure, much less the electronic behavior across a surface, is poor. We present a systematic approach for computing surface structure and energies that resolves remaining limitations in density functional theory calculations of surface properties. The methods are established in validated Aluminum surface studies, and then detailed calculations for various reconstructed low-index surfaces for Platinum provide new explanations into observed surface reconstructions and seemingly anomalous growth behavior, and gives new insight into possible emission behavior interpreted in terms of a local work function. The implication of these results are interpreted in terms of models of electron emission and surface measurements with STM, as a foundation of a multiscale approach to understanding and modeling vacuum breakdown for grown Pt surfaces.

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