

Metallic surfaces in the ThomasFermivon Weizsäcker approach: Self-consistent solution

Utreras-Diaz, Constantino A.

The problem of a metallic surface is studied and solved in the ThomasFermivon Weizsäcker approach. The analysis of the asymptotic solutions shows that the electronic density $n(x)$ approaches its bulk value n_0 in the metal interior exponentially, oscillating about it. This behavior is found to be an effect of the von Weizsäcker term, rather than of the exchange-correlation interaction, as one may have thought. The Euler equation is solved for a slab geometry, calculating work functions and surface energies of several simple metals. The case of the pseudojellium model, recently introduced, is also considered here. The results are compared with those of the exact Lang-Kohn theory and with those of Smith. © 1987 The American Physical Society.