

Surface Energy of Jellium: Was Density Functional Theory Right All Along?

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The surface energy or surface tension is the work required to cut a unit area of new surface. In 1970, Lang and Kohn used the local density approximation (LDA) to calculate the surface energy for jellium and real metals. The apparent success of their effort stimulated interest in why this approximation worked and how to improve it. But subsequent calculations with correlated wavefunctions suggested that the LDA surface energies are seriously too low. I will discuss three sophisticated density functional calculations, plus a new way to extract surface energies from Diffusion Monte Carlo energies of jellium spheres, which all suggest that the LDA surface energies were nearly right after all.