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High-Level Correlated Approach to the Jellium Surface Energy, Without Uniform-Electron-Gas Input[1] LUCIAN CONSTANTIN, Tulane University, LUCIAN CONSTANTIN COLLABORATION, J.M. PITARKE COLLABORATION, J.F. DOBSON COLLABORATION, A. GARCIA-LEKUE COLLABORATION, J.P. PERDEW COLLABORATION — We resolve the long-standing controversy over the surface energy of simple metals: Density functional methods that require uniform-electron-gas input agree with each other at many levels of sophistication, but not with high-level correlated calculations like Fermi Hypernetted Chain and Diffusion Monte Carlo (DMC) that predict the uniform-gas correlation energy. Here we apply a very high-level correlated approach, the inhomogeneous Singwi-Tosi-Land-Sjölander (ISTLS) method, and find that the density functionals are indeed reliable (because the surface energy is "bulk-like"). ISTLS values are close to recently-revised DMC values. Our work also vindicates the previously-disputed use of uniform-gas-based nonlocal kernels in time-dependent density functional theory.

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