Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Correlation effects in metallic cohesion[1] ROGER HAYDOCK, University of Oregon — The electronic contribution to the cohesive energy of a correlated metal is the sum of the transition energies for adding successive electrons at successive Fermi levels until the system reaches its final electron density. This can be computed as the integral of energy over the projected density of transitions for adding single electrons to localized orbitals. In the case of independent electrons, this reduces to the usual integral over the projected density of states. As an example, cohesive energies for some simple transition metal structures are calculated using the recursion method* with a Hubbard repulsion between electrons. * Phys. Rev. B 61, 7953-64

[1]Work supported by the Richmond F. Snyder gift to the University of Oregon

Roger Haydock
University of Oregon

Date submitted: 14 Nov 2013 Electronic form version 1.4