Electronic correlation contributions to structural energies

ROGER HAYDOCK, University of Oregon — The recursion method is used to calculate electronic excitation spectra including electron-electron interactions within the Hubbard model. The effects of correlation on structural energies are then obtained from these spectra and applied to stacking faults. http://arxiv.org/abs/1405.2288

1Supported by the Richmond F. Snyder Fund and Gifts

Roger Haydock
University of Oregon

Date submitted: 13 Nov 2014