Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Electronic and Structural Properties of Chains of Metals MICHAEL SPRINGBORG, YI DONG, ABU ASSADUZZAMAN, University of Saarland, Saarbruecken, Germany — We report results of parameter-free calculations of the structural and electronic properties of isolated metal chains. The calculations have been performed using our own density-functional methods that has been developed for isolated, infinite, periodic, helical chains with a straight chain axis. We study linear, zigzag, double-zigzag, and tetragonal chains of Au, Ag, Al, Pt, Bi, Pb, and Tl, and discuss the relative stability of the different forms, distortion modes, effects of spin-orbit couplings, and band structures.

Michael Springborg
University of Saarland, Saarbruecken, Germany

Date submitted: 22 Nov 2004 Electronic form version 1.4