

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

A Robust Spectrum Slicing Method Applied to the Kohn-Sham Equation for the Liquid/Solid Silicon Interface¹ GRADY SCHOFIELD, JAMES CHELIKOWSKY, University of Texas at Austin — A difficult aspect of solving the Kohn Sham equation is the super-linear scaling of eigensolvers with the number of valence orbitals desired. We present a robust spectrum slicing technique that calculates the valence orbitals in a divide and conquer fashion through the use of smooth Chebyshev-Jackson filters. This algorithm allows for a “parallel” implementation of the eigensolver. Our calculations are done in the real-space density functional framework implemented in the program PARSEC. We apply this method to examine the liquid-solid silicon interface.

¹Supported by the National Science Foundation OCI-1047997, DMR-0941645 and the Welch Foundation (F-1708)

Grady Schofield
University of Texas at Austin

Date submitted: 17 Nov 2010

Electronic form version 1.4