Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

A Computational Method for Materials Design of New Interfaces JAKUB KAMINSKI, CHRISTIAN RATSCH, University of California Los Angeles, JUSTIN WEBER, MICHAEL HAVERTY, Intel Corporation, SADASIVAN SHANKAR, formerly Intel Corporation — We propose a novel computational approach to explore the broad configurational space of possible interfaces formed from known crystal structures to find new heterostructure materials with potentially interesting properties. In a series of steps with increasing complexity and accuracy, the vast number of possible combinations is narrowed down to a limited set of the most promising and chemically compatible candidates. This systematic screening encompasses (i) establishing the geometrical compatibility along multiple crystallographic orientations of two materials, (ii) simple functions eliminating configurations with unfavorable interatomic steric conflicts, (iii) application of empirical and semi-empirical potentials estimating approximate energetics and structures, (iv) use of DFT based quantum-chemical methods to ascertain the final optimal geometry and stability of the interface in question. For efficient high-throughput screening we have developed a new method to calculate surface energies, which allows for fast and systematic treatment of materials terminated with non-polar surfaces. We show that our approach leads to a maximum error around 3% from the exact reference. The representative results from our search protocol will be presented for selected materials including semiconductors and oxides.

Jakub Kaminski
University of California Los Angeles

Date submitted: 14 Nov 2014 Electronic form version 1.4