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A Computational Method for Materials Design of Interfaces JAKUB KAMINSKI, CHRISTIAN RATSCH, Department of Mathematics, University of California Los Angeles, SADASIVAN SHANKAR, Design and Technology Solutions, Technology and Manufacturing Group, Intel Corporation — In the present work we propose a novel computational approach to explore the broad configurational space of possible interfaces formed from known crystal structures to find new hetrostructure materials with potentially interesting properties. In the series of subsequent 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 (or more) 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. We also demonstrate the flexibility and efficiency of our approach depending on the size of the investigated structures and size of the search space. The representative results from our search protocol will be presented for selected materials including semiconductors, transition metal systems, and oxides.

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