Abstract Submitted
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Improvements to the NRL Tight-Binding Model[1] MICHAEL MEHL, Naval Research Laborator, DIMITRIOS PAPACONSTANTOPOULOS, George Mason University, NOAM BERNSTEIN, Naval Research Laboratory, DANIEL FINKENSTADT, United States Naval Academy, STEFANO CURTAROLO, Duke University — The original NRL Tight-Binding Method[1] has proven to be extremely successful in reproducing first-principles total energies and band structures for many elemental systems[2], and has been applied in computationally intensive molecular dynamics simulations[3]. When generalizing to multiple atom types, however, some difficulties arise because of the form of the interaction of the on-site matrix elements with the external environment. We discuss these difficulties, and describe a new version of the method which includes a proper two-center development of the on-site parameters[4,5], including applications of the method. [1] RE Cohen et al., Phys. Rev. B 50, 14694 (1994) [2] MJ Mehl and DA Papaconstantopoulos, Phys. Rev. B 54, 4519 (1996) [3] D Finkenstadt et al., Phys. Rev. B 74, 184118 (2006) [4] JL Mercer and MY Chou, Phys. Rev. B 49, 8506 (1994) [5] RE Cohen et al., Phys. Rev. B 56, 8575 (1997)

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