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**Tight-binding Hamiltonian for LaFeAsO** DIMITRIOS PAPACONSTANTOPOULOS, LANE NIXON, George Mason University, MICHAEL MEHL, Naval Research Laboratory — There have been several first-principles calculations reported recently for the superconducting pnictinide LaFeAsO and related compounds. In addition, tight-binding(TB) Hamiltonians for these systems have been constructed with varying degrees of success. In this work we have used the NRL-TB method to fit our LAPW results to a TB basis with the aim of reproducing the band structure very accurately. We have included the s and d orbitals of Fe, the s and p orbitals of As, and the p orbitals of O. We present a study of these TB results in terms of the effect of each of the above orbitals on how accurately the first-principles band structure can be reproduced. Finally, we assess the feasibility of carrying out many-body theory with a Hamiltonian that may contain more than just the d-Fe orbitals.

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