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Tight-binding Hamiltonian for LaFeAsO[1] D. A. PAPACONSTANTOPOULOS, George Mason University, Fairfax VA, MICHAEL MEHL, MICHELLE JOHANNES, DAVID PARKER[2], Naval Research Laboratory, Washington DC — We construct a realistic tight-binding Hamiltonian (TB) fitted to first-principles band structure calculations of the pnictide parent compound LaFeAsO. We have come to the conclusion that most previously derived (TB) Hamiltonians poorly reproduce the first-principles results. Here we use the NRL-TB method to fit our LAPW results as a function of volume and As displacement. The TB basis includes the Fe d, As p, and O p-orbitals. We omit the La d-orbitals, which only contribute to states well above the Fermi level. We find a TB band structure that fits an LAPW range of energies with a width of 3.5 eV. The bands near the Fermi level fit the LAPW results very well, reproducing the Fermi surface near Γ and M. The TB densities of states agree with first-principles results. We also study the variation of the total energy with respect to the position of the As atoms. We find that the TB total energies fit the LAPW values very well even for structures not included in our fit. We use our accurate hopping parameters to uncover the origin of the so far unexplained pseudogap near the Fermi energy and explore the evolution of this gap with magnetism.

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