

Abstract Submitted
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Development of a Semi-empirical Hamiltonian for Phosphorus for Quantum Mechanics Based Simulations of Phosphorous-based Nanostructures PAUL TANDY, CHRISTOPHER LEAHY, MING YU, C.S. JAYANTHI, S.Y. WU, University of Louisville — We have developed a parameterized semi-empirical Hamiltonian for phosphorous for simulation studies of phosphorous-based nanostructures including phosphorous-doped silicon nanowires. This Hamiltonian models the environment-dependent electron-ion and ion-ion interactions and electron-electron correlations, by capturing the salient features of *ab initio* Hamiltonians/*ab initio* methods, (*e.g.*, electron screening and charge self-consistency). Such a semi-empirical Hamiltonian has been shown to be successful in predicting the properties of intermediate-sized silicon, boron, and carbon clusters and extended structures of boron and silicon [1-4]. We optimized the parameters of our Hamiltonian for phosphorous by fitting the properties of bulk (black phosphorous) and small clusters (P_2 to P_{10}) as obtained by our method to *ab initio* calculations. It is expected that such a Hamiltonian will have the predictive power to enable the study of larger phosphorous based nanostructures that are not possible via *ab initio* studies.

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