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Full-scope modeling of semiconductor devices for quantum information processing JOHN KING GAMBLE, ANDREW BACZEWSKI, Sandia National Labs, ADAM FREES, University of Wisconsin-Madison, N. TOBIAS JACOBSON, INES MONTANO, RICHARD P. MULLER, ERIK NIELSEN, Sandia National Labs — Recent outstanding experimental advances in semiconductor-based quantum information processing have placed the fundamental building blocks of a quantum computer within reach. Typical computational simulation of these devices either focuses on the large-scale, semiclassical device physics or more detailed quantum mechanics within an idealized physical system. Here, we present results for full-scope simulation, where detailed multi-valley effective mass theory is coupled to large-scale device physics. This enables the simulation of the quantum properties and operation of a device directly from a physical design. This work opens the door for physics-targeted device optimization and an unprecedented level of predictive power. The authors gratefully acknowledge support from the Sandia National Laboratories Truman Fellowship Program, which is funded by the Laboratory Directed Research and Development (LDRD) Program. Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the US Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

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