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Sifting Through Data from a Two Donor Simulation in Silicon[1] ANDRE SARAIVA, IF-UFRJ, M. FERNANDO GONZALEZ-ZALBA, Hitachi Cambridge Laboratory, DOMINIK HEISS, Cavendish Laboratory, MARIA CALDERÓN, ICMM-CSIC, BELITA KOILLER, IF-UFRJ, ANDREW FERGUSON, Cavendish Laboratory, JUAN DEHOLLAIN, JUHA MUHONEN, KUAN TAN, DAVID JAMIESON, ANDREW DZURAK, ANDREA MORELLO, Centre for Quantum Computation and Communication Technology, ALEJANDRA BAENA, IF-UFRJ — Recently, two independent demonstrations of exchange-coupled donor pairs [1,2] have provided an early step towards two spin entanglement. Even though these systems are not yet suitable for quantum computation, they make blatant the need for more thorough theoretical investigation and, more importantly, more efficient surveying of the large dataset generated by the numerical investigations. We will discuss how useful information can be extracted from large datasets obtained with full configuration interaction, multivalley, central-cell corrected effective mass calculations [3]. As examples, we will study the successful cases of theory-experiment comparison in Refs. [1] and [2], as well as provide early predictions for other systems, such as singlet-triplet donor-based qubits. [1] M. F. Gonzalez-Zalba, A. Saraiva, D. Heiss, M. J. Calderón, B. Koiller, and A. J. Ferguson, arXiv:1312.4589 (2013) [2] J. P. Dehollain, J. T. Muhonen, K. Y. Tan, A. Saraiva, D. N. Jamieson, A. S. Dzurak, and A. Morello, Phys. Rev. Lett. 112, 236801 (2014). [3] A. L. Saraiva, A. Baena, M. J. Calderón, and B. Koiller, arXiv:1407.8224 (2014)

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