

Codoped Quantum Dots as Qubits

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Quantum dots have the potential to be used for quantum computation.¹ Here we are developing a theoretical and computational model to use two coupled codoped quantum dots to implement two qubits and an elementary quantum gate. An atomistic model of a codoped silicon quantum dot with composition $\text{Al}_1\text{P}_1\text{Si}_{36}\text{H}_{42}$ was created for the computational treatment. We extract parameters from the quantum dot model using semi-empirical methods and time-dependent density functional theory.² Parameters computed by quantum chemical methods, such as energies of states ε_i for each qubit and the system coupling V , are used for the theoretical model. Originally, the qubits are isolated, but are brought together to allow interaction. In the case of quantum dots, this is done with the help of an external electric field. V is computed for various distances between quantum dots and for various strengths of the electric field. The value of the coupling V determines the level splitting and information transfer between the qubits during this interaction. The splitting of energies shows transition from quadratic to linear dependence in limits of small and large values of V . This model parametrization is applied to the time-dependent Schrodinger equation for the system, which we are currently solving. Through the solution we find the time dependent expansion coefficients of the wavefunction in the basis of molecular orbital's $c_{\alpha\alpha}(t)$, $c_{\alpha\beta}(t)$, $c_{\beta\alpha}(t)$, $c_{\beta\beta}(t)$, for various initial conditions. This solution allows us to analyze the controlled transfer of quantum population and superposition between parts of the model representing the two qubits.

References

1. (a) Loss, D.; DiVincenzo, D. P., Quantum computation with quantum dots. *Physical Review A* **1998**, 57 (1), 120-126; (b) Norris, D. J.; Efros, A. L.; Erwin, S. C., Doped nanocrystals. *Science* **2008**, 319 (5871), 1776-1779.
2. Mavros, M. G.; Micha, D. A.; Kilin, D. S., Optical Properties of Doped Silicon Quantum Dots with Crystalline and Amorphous Structures. *J. Phys. Chem. C* **2011**, 115 (40), 19529-19537.

D.K. acknowledges the NSF award EPS0903804 and allocation award 84577 with NERSC contract No. DE-AC02-05CH11231