20th Brazilian Workshop on Semiconductor Physics

Investigation of electrically controlled charge Qubit in van der Waals heterostructures: a tight-binding approach

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Abstract

The development of quantum mechanics has led to a deeper understanding of fundamental aspects of matter and radiation and has been the basis of many emerging technologies. In particular, the possibility of utilizing quantum processes to develop a quantum computer (QC) represents a paradigm shift in computation. By exploiting the natural parallelism of the evolution of quantum states, QCs are expected to surpass the performance of their classical counterparts. The superior performance of QCs could help tackle problems such as drug development, disease predictions, simulation of complex systems such as molecules, and new types of cryptographic encryption, and significantly improve machine learning and artificial intelligence technologies. However, recent developments in QC hardware have focused on using superconducting qubits, which operate at cryogenic temperatures. Thus, there has been a strong interest in developing qubits that are both robust and can operate at higher temperatures.

In this work, we investigate the implementation of a charge qubit in van der Waals heterostructures [1] following an approach based on a tight-binding (TB) model, within the formalism of Marzari and Vanderbilt [2,3], obtained from ab initio calculations within the DFT (density functional theory). First, a DFT investigation of over 20 monolayers was performed to analyze and select those with favorable characteristics for a charge qubit. Then, the control of the hybridized states is analyzed via the TB model with a low computational cost keeping the hoppings fixed and the onsite energies being perturbed via an electric potential. The model was shown consistent with previous DFT calculations, thus being validated. Further, this approach can be generalized to other systems, given the possibility of studying the transport of these new qubits.

References

1. Bruno Lucatto et. al, Phys. Rev. B 100 (R), 121406 (2019)
2. N. Marzari and D. Vanderbilt, Phys. Rev. B 56, 12847 (1997)
3. I. Souza, N. Marzari and D. Vanderbilt, *Phys. Rev. B* **65**, 035109 (2002)