Abstract Submitted for the MAR07 Meeting of The American Physical Society

Electronic structure, entanglement and double occupancy in asymmetric dot molecule quantum gate¹ LIXIN HE, Key Laboratory of Quantum Information, USTC, Hefei, Anhui, 230026, P.R. China, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, Colorado 80401, USA — First, we describe the energy levels, degree of entanglement and double occupancy in fully symmetric (homopolar) quantum dot molecules (QDM) made of InGaAs dots in a GaAs barrier containing $\sim 3 \times 10^6$ atoms. We describe the single-particle part by atomistic pseudopotential theory including strain and alloy effects, and the many body part via configuration interaction. Second, we note that in a realistic vertically coupled QDM the two dots often have different geometries, sizes, alloy compositions, (heteropolar QDM) and therefore, deviates from ideal homopolar QDM model used previously. We show that the electronic properties of such heteropolar QDMs are greatly modified by the asymmetry of the QDMs, showing larger two-electron double occupation rate, lower two-electron entanglement, and therefore reduced quantum gate quality. By symmetrizing the QDM via application of electric field, one can overcome these difficulties.

¹Supported by Chinese NSF Grant No. 60121503 and US.

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Date submitted: 19 Nov 2006

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