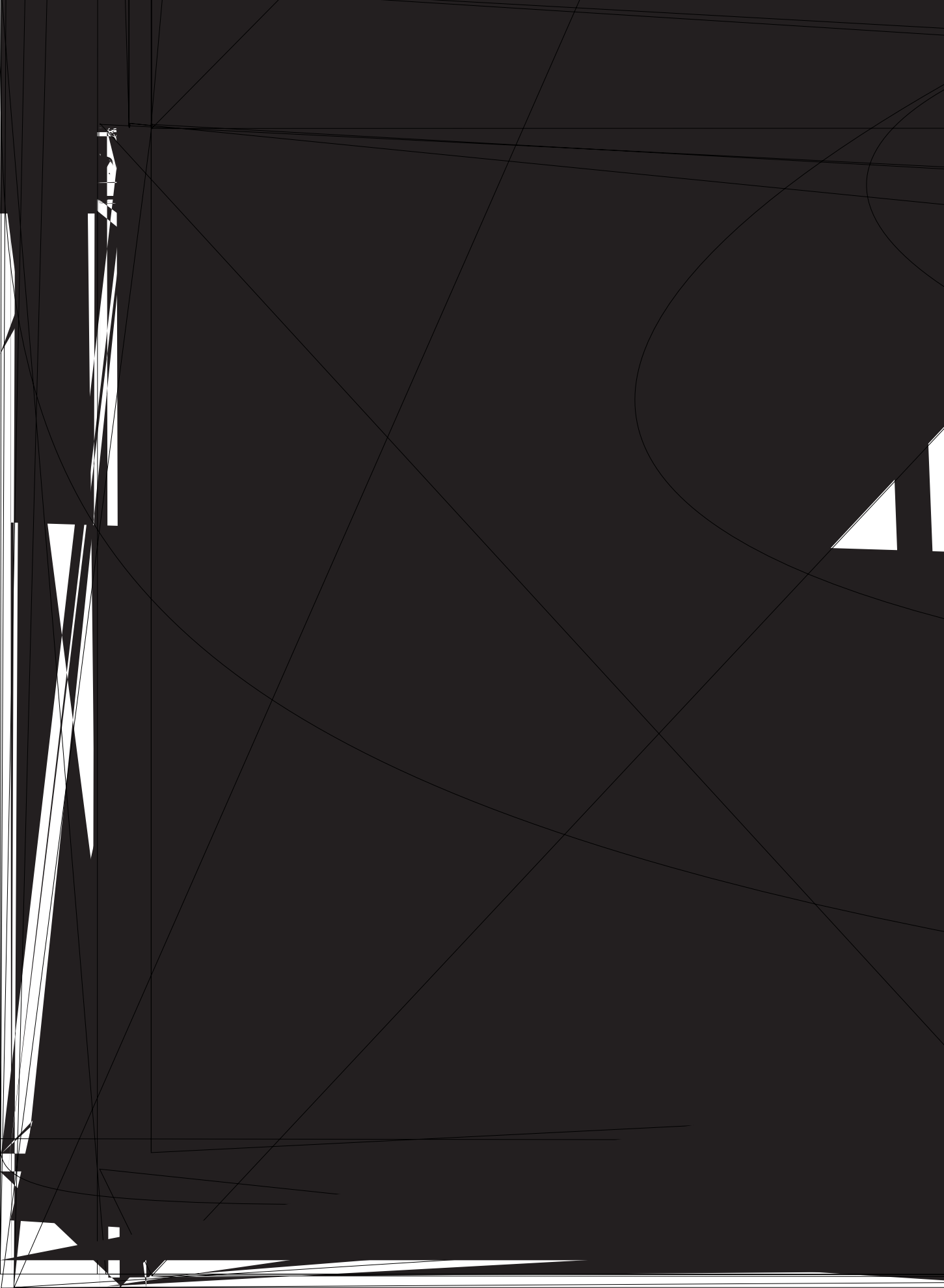
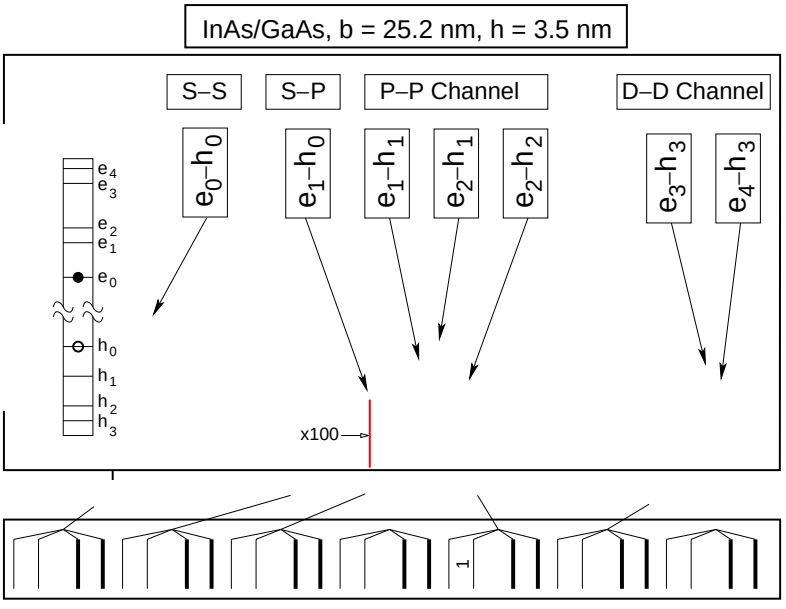
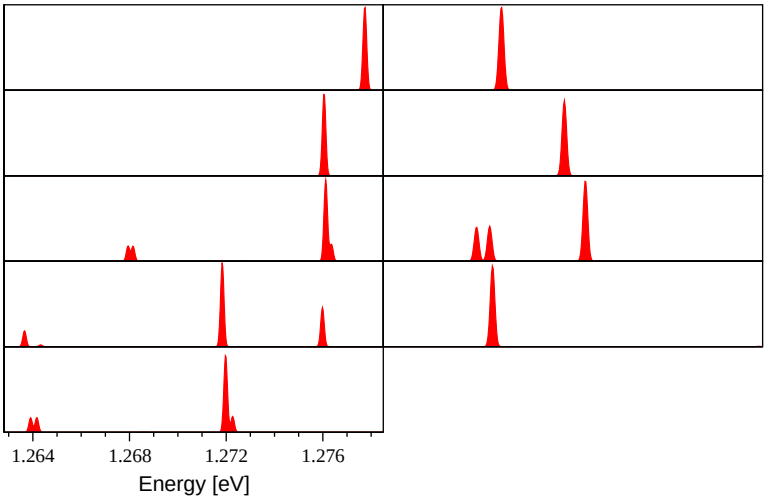


and featureless envelope functions $F_n(\ )$ cannot properly resolve the atomistic detail of the object being modeled. Thus, the theory is "hyperopic", seeing the global shape but not the detailed symmetry. This was demonstrated recently in Ref. [12], where k:p was shown to miss the correct symmetry of dots, leading to], where


InAs/GaAs, b = 25.2 nm, h = 3.5 nm
S–S
S–P
P–P Channel
D–D Channel
e0–h0
e1–h0
e1–h1
e2–h1
e2–h2
e3–h3
e4–h3
e4
e3
e2
e1
e0
h0
h1
h2
h3
x100
1


1.264
1.268
1.272
1.276
Energy [eV]

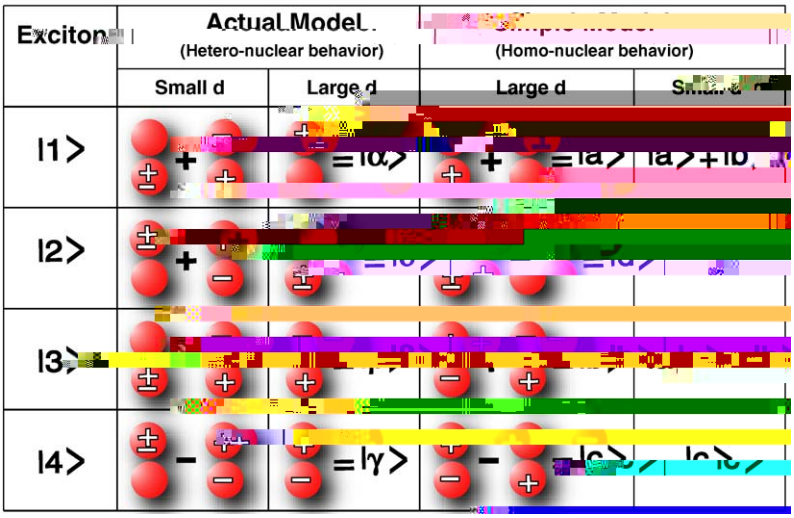


Fig. 5. Schematic representation of the excitonic wave functions obtained in our model (left), and in the simple model of Bayer et al. [38] (right). The symbols are: +(hole), −(electron) or ±(exciton). The two spheres denote top and bottom dots.

The excitonic spectra we calculated for our dot molecules are shown in Fig. 4(d) and is very di□erent from the simple model. Our dots are 12 nm × 2 nm truncated-cone-shaped dots, with a linear composition gradient varying from $In_{0:5}Ga_{0:5}As$ at their bases to pure InAs at their tops. In Fig. 4(d) the oscillator strength of the □rst four excitons $|1\rangle$, $|2\rangle$, $|3\rangle$ and $|4\rangle$ is proportional to the size of the circles. We see (i) at large inter-dot separations only the □rst two excitons $|1\rangle$ and $|2\rangle$ are optically allowed, corresponding to excitons where the electron–hole pair is localized to the top and bottom dot, respectively. In contrast, the excitons $|1\rangle$ and $|3\rangle$ are optically allowed in the simple model. The dots are geometrically identical but due to random alloy □uctuations present in real dots, and taken into account in our calculations, the top dot is preferred by the exciton (see Fig. 5). The "dissociated states" $|3\rangle$ and $|4\rangle$, where the electron and the hole resides on di□erent dots have no oscillator strength since there is no e–h overlap. (ii) At small inter-dot separation there are four states, all dipole-allowed. This is due to the interaction of the four excitons $|1\rangle$, $|2\rangle$, $|3\rangle$ and $|4\rangle$ which mix, like shown in Fig. 5. All four excitons are mixed excitonic-dissociated states with non-zero oscillator strength. (iii) At large inter-dot separation, the exciton states $|1\rangle$ and $|2\rangle$ and the dissociated states $|3\rangle$ and $|4\rangle$ are separated by about 20 meV.

(iv) The lines collapse into one at a special separation of 8:5 nm. At this separation the entanglement (that can be calculated from our CI wave functions, following the de□nition of Von Neumann [39,40]) reaches a maximum of 80%. The degree of entanglement sharply drops for larger and shorter inter-dot separations (not shown).

R

[1] E. Kane, J. Phys. Chem. Sol. 1 (1957) 249.
[2] J. Luttinger, W. Kohn, Phys. Rev 97 (1955) 869.
[3] G. Bara□, D. Gershoni, Phys. Rev. B 43 (1991) 4011.
[4] G. Bastard, Wave Mechanics Applied to Semiconductor Heterostructures, Halstead, New York, 1988.
[5] M. Cardona, F. Pollak, Phys. Rev 142 (1966) 530.
[6] A. Franceschetti, S. Wei, A. Zunger, Phys. Rev. B 50 (1994) 8094.
[7] A. Franceschetti, S. Wei, A. Zunger, Phys. Rev. B 52 (1995) 13992.
[8] H. Fu, L. Wang, A. Zunger, Phys. Rev. B 57 (1998) 9971.
[9] H. Fu, L. Wang, A. Zunger, Appl. Phys. Lett. 73 (1998) 1157.
[10] L. Wang, A. Zunger, Phys. Rev. B 54 (1996) 11417.
[11] D. Wood, A. Zunger, Phys. Rev. B 53 (1996) 7949.
[12] A. Zunger, Phys. Stat. Sol. (A) 190 (2002) 467.

[13] L.-W. Wang, A. Zunger, Phys. Rev. B 59 (1999) 15806.
[14] A. Franceschetti, et al., Phys. Rev. B 60 (1999) 1819.
[15] G. Bester, S.V. Nair, A. Zunger, Phys. Rev. B 67 (2003) 161306.
[16] M. Bayer, et al., Phys. Rev. Lett. 82 (1999) 1748.
[17] M. Bayer, et al., Phys. Rev. B 65 (2002) 195315.
[18] T. Walther, et al., Phys. Rev. Lett. 86 (2001) 2381.
[19] R. Kegel, P.M. Petro□, et al., Phys. Rev. B 63 (2001) 035318.
[20] Y. Ducommun, et al., Phys. Stat. Sol. (B) 224 (2001) 325.
[21] U. Hohenester, E. Molinari, Phys. Stat. Sol. (B) 221 (2000) 19.
[22] D.V. Regelman, et al., Physica E 13 (2002) 114.
[23] R.J. Warburton, et al., Phys. Rev. B 58 (1998) 16221.
[24] R.J. Warburton, et al., Nature 405 (2000) 926.
[25] R.J. Warburton, et al., Physica E 9 (2001) 124.
[26] J.J. Finley, et al., Phys. Rev. B 63 (2001) 161305.
[27] G. Bester, A. Zunger, Phys. Rev. B 68 (2003) 073309.
[28] A. Ashmore, et al., Physica E 13 (2002) 127.
[29] M. Baier, et al., Phys. Rev. B 64 (2001) 195326.
[30] F. Findeis, et al., Appl. Phys. Lett. 78 (2001) 2958.
[31] F. Findeis, et al., Phys. Rev. B 63 (2001) 121309.
[32] A. Hartmann, et al., Phys. Rev. Lett. 84 (2000) 5648.
[33] K. Karlsson, E. Moskalenko, P. Holtz, B. Monemar, W. Schoenfeld, J. Garcia, P. Petro□, Physica E 13 (2002) 101.
[34] K.F. Karlsson, et al., Acta. Phys. Pol. 100 (2001) 387.
[35] D.V. Regelman, et al., Phys. Rev. B 64 (2001) 165301.
[36] A. Zrenner, et al., Physica E 13 (2002) 95.
[37] P.W. Fry, et al., Phys. Rev. Lett. 84 (2000) 733.
[38] M. Bayer, et al., Science 291 (2001) 451.
[39] C.H. Bennett, D.P. DiVincenzo, Nature 404 (2000) 247.
[40] M.A. Nielsen, I.L. Chuang, Quantum Computation and Quantum Information, Cambridge University Press, Cambridge, 2000.