TABLES

TABLE I. Experimental and fitted bulk InAs pseudopotential properties. Δ_{SO} is the spin-orbit splitting and $m^*_{\Gamma_{1c}}$, $m^*_{\Gamma_{15v},hh}$ and $m^*_{\Gamma_{15v},lh}$ are the effective masses of electrons, heavy and light holes.

Property	Expt. Value	Pseudopotential
Γ_{1c}	0.42	0.41
X_{1c}	2.33	2.27
L_{1c}	1.71	1.61
Δ_0	0.38	0.36
$m^*_{\Gamma_{1c}}$	0.029	0.028
$m^*_{\Gamma_{15v},hh}[100]$	0.43	0.41
$m^*_{\Gamma_{15v},lh}[100]$	0.038	0.039

TABLE II. InAs quantum dot sizes and compositions

Dot Number	1	2	3	4
No. In atoms	140	276	456	736
No. As atoms	141	249	459	683
Diameter (Å)	23.9	30.3	36.6	42.2

TABLE III. Contributions (as fractions of unity) from the split-off (SO), heavy hole (hh), light hole (lh) and conduction band (CBM) bulk states to the single particle states of the InAs dot with 23.9Å diameter. The dot states are numbered (first column) from the band edge. For electron states 1 is the lowest in energy, 8 the highest. For hole states, 1 is the highest in energy, 24 the lowest. The contribution from each state is determined using Eq.(8). For each state the bulk SO, hh+lh and CBM contributions are decomposed into their angular momentum components using Eq.(10). Only the states contributing to the major excitonic peaks in Fig. 8 are shown. All entries less than 0.01 are set to 0.0. The main contributions are marked in bold. Totals include envelope functions with angular momenta from 0 to 6.

		SO Contribution				hh + lh Contribution				CBM Contribution			
Level	Energy (eV)	s	p	d	Total	s	p	d	Total	s	p	d	Total
Conduction States													
1	ϵ_c	0.	0.07	0.	0.07	0.	**0.17**	0.	**0.17**	**0.65**	0.01	0.000	**0.66**
6,7	$\epsilon_c + 0.442$	0.01	0.	0.03	0.05	0.02	0.	0.06	0.09	0.01	**0.45**	0.01	**0.51**
8	$\epsilon_c + 0.444$	0.	0.	0.05	0.05	0.03	0.	0.05	0.09	0.000	**0.37**	0.01	**0.43**
Valence States													
1,2	ϵ_v	0.01	0.01	0.02	0.06	**0.45**	**0.22**	**0.11**	**0.83**	0.	0.01	0.01	0.02
3,4	$\epsilon_v - 0.065$	0.01	0.01	0.01	0.05	0.02	**0.39**	**0.26**	**0.81**	0.	0.	0.	0.
5,6	$\epsilon_v - 0.131$	**0.36**	**0.28**	0.03	**0.60**	0.01	**0.10**	**0.10**	**0.21**	0.	0.01	0.01	0.02
9,10	$\epsilon_v - 0.214$	0.	0.04	0.03	0.14	0.02	**0.19**	**0.12**	**0.64**	0.	0.	0.	0.
12,13	$\epsilon_v - 0.266$	0.	0.01	0.02	0.06	**0.11**	**0.27**	**0.15**	**0.83**	0.	0.	0.	0.
14,15	$\epsilon_v - 0.342$	0.02	0.04	0.03	**0.18**	0.	0.09	0.08	**0.42**	0.	0.	0.	0.

TABLE IV. Contributions (as fractions of unity) from the split-off (SO), heavy hole (hh), light hole (lh) and conduction band (CBM) bulk states to the single particle states of the InAs dot with 30.3Å diameter. The dot states are numbered (first column) from the band edge. For electron states 1 is the lowest in energy, 8 the highest. For hole states, 1 is the highest in energy, 24 the lowest. The contribution from each state is determined using Eq.(8). For each state the bulk SO, hh+lh and CBM contributions are decomposed into their angular momentum components using Eq.(10). Only the states contributing to the major excitonic peaks in Fig. 8 are shown. All entries less than 0.01 are set to 0.0. The main contributions are marked in bold. Totals include envelope functions with angular momenta from 0 to 6.

		SO Contribution				hh + lh Contribution				CBM Contribution			
Level	Energy (eV)	s	p	d	Total	s	p	d	Total	s	p	d	Total
Conduction States													
1	ϵ_c	0.05	0.05	0.000	0.10	**0.10**	**0.13**	0.	**0.23**	**0.50**	0.05	0.	**0.55**
6,	$\epsilon_c + 0.444$	0.	0.05	0.04	0.09	0.06	**0.10**	0.05	**0.21**	0.	**0.42**	0.04	**0.47**
7,8	$\epsilon_c + 0.446$	0.01	0.05	0.03	0.09	0.03	0.09	0.07	**0.19**	0.02	**0.41**	0.03	**0.47**
Valence States													
1,2	ϵ_v	0.	0.	0.03	0.03	**0.61**	0.03	0.07	**0.71**	0.	0.03	0.01	0.04
3,4	$\epsilon_v - 0.038$	0.	0.02	0.01	0.04	0.03	**0.58**	0.01	**0.64**	0.	0.04	0.	0.04
5,6	$\epsilon_v - 0.126$	**0.37**	0.	0.	**0.39**	0.	**0.13**	**0.13**	**0.29**	0.03	0.02	0.02	0.08
7,8	$\epsilon_v - 0.138$	0.	0.07	0.	0.10	0.	**0.32**	0.07	**0.50**	0.	0.04	0.03	0.09
12,13	$\epsilon_v - 0.196$	0.	0.01	0.02	0.06	**0.23**	0.05	**0.18**	**0.53**	0.04	0.01	0.02	0.08
15	$\epsilon_v - 0.262$	**0.22**	0.01	0.	**0.27**	0.	0.03	**0.22**	**0.38**	0.01	0.01	0.02	0.06
17,18	$\epsilon_v - 0.270$	0.	0.08	0.01	0.11	0.01	**0.30**	0.13	**0.69**	0.	0.01	0.01	0.03
23,24	$\epsilon_v - 0.332$	0.	0.04	0.01	0.10	0.	**0.23**	0.07	**0.52**	0.	0.02	0.02	0.06

TABLE V. Contributions (as fractions of unity) from the split-off (SO), heavy hole (hh), light hole (lh) and conduction band (CBM) bulk states to the single particle states of the InAs dot with 36.9Å diameter. The dot states are numbered (first column) from the band edge. For electron states 1 is the lowest in energy, 8 the highest. For hole states, 1 is the highest in energy, 24 the lowest. The contribution from each state is determined using Eq.(8). For each state the bulk SO, hh+lh and CBM contributions are decomposed into their angular momentum components using Eq.(10). Only the states contributing to the major excitonic peaks in Fig. 8 are shown. All entries less than 0.01 are set to 0.0. The main contributions are marked in bold. Totals include envelope functions with angular momenta from 0 to 6.

		SO Contribution				hh + lh Contribution				CBM Contribution			
Level	Energy (eV)	s	p	d	Total	s	p	d	Total	s	p	d	Total
Conduction States													
1	ϵ_c	0.	0.07	0.	0.07	0.	**0.20**	0.	**0.20**	**0.68**	0.	0.	**0.68**
2	$\epsilon_c + 0.392$	0.06	0.	0.	0.06	0.	0.	**0.17**	**0.17**	0.	**0.60**	0.01	**0.61**
3,4	$\epsilon_c + 0.404$	0.	0.	0.07	0.07	0.08	0.	0.09	**0.17**	0.	**0.61**	0.01	**0.62**
Valence States													
1,2	ϵ_v	0.	0.01	0.03	0.04	**0.70**	0.06	**0.11**	**0.87**	0.	0.03	0.	0.03
3,4	$\epsilon_v - 0.023$	0.	0.02	0.01	0.04	0.04	**0.76**	0.04	**0.90**	0.	0.	0.01	0.01
5,6	$\epsilon_v - 0.117$	0.	0.07	0.02	0.13	0.01	**0.33**	**0.25**	**0.78**	0.	0.	0.01	0.01
11,12	$\epsilon_v - 0.151$	0.	0.	0.02	0.05	**0.37**	0.04	**0.30**	**0.83**	0.	0.01	0.	0.01
15	$\epsilon_v - 0.217$	**0.25**	0.	0.	**0.29**	0.	**0.10**	**0.27**	**0.43**	0.	0.01	0.	0.02
16,17	$\epsilon_v - 0.234$	0.	**0.11**	0.07	**0.21**	0.04	0.07	0.06	**0.63**	0.	0.	0.	0.
23,24	$\epsilon_v - 0.272$	0.	0.08	0.	0.14	0.01	**0.32**	**0.11**	**0.69**	0.	0.	0.01	0.01

TABLE VI. Contributions (as fractions of unity) from the split-off (SO), heavy hole (hh), light hole (lh) and conduction band (CBM) bulk states to the single particle states of the InAs dot with 42.2Å diameter. The dot states are numbered (first column) from the band edge. For electron states 1 is the lowest in energy, 8 the highest. For hole states, 1 is the highest in energy, 24 the lowest. The contribution from each state is determined using Eq.(8). For each state the bulk SO, hh+lh and CBM contributions are decomposed into their angular momentum components using Eq.(10). Only the states contributing to the major excitonic peaks in Fig. 8 are shown. All entries less than 0.01 are set to 0.0. The main contributions are marked in bold. Totals include envelope functions with angular momenta from 0 to 6.

		SO Contribution				hh + lh Contribution				CBM Contribution			
Level	Energy (eV)	s	p	d	Total	s	p	d	Total	s	p	d	Total
Conduction States													
1	ϵ_c	0.	0.07	0.	0.07	0.	**0.20**	0.	**0.20**	**0.69**	0.	0.	**0.69**
2	$\epsilon_c + 0.360$	0.06	0.	0.01	0.07	0.01	0.	**0.19**	**0.20**	0.	**0.64**	0.01	**0.65**
3,4	$\epsilon_c + 0.361$	0.	0.	0.07	0.07	0.09	0.	**0.10**	**0.19**	0.	**0.64**	0.01	**0.65**
Valence States													
1,2	ϵ_v	0.	0.02	0.02	0.04	**0.50**	**0.29**	0.09	**0.89**	0.	0.02	0.	0.02
3,4	$\epsilon_v - 0.014$	0.	0.01	0.01	0.03	**0.23**	**0.55**	0.07	**0.88**	0.	0.01	0.	0.01
7,8	$\epsilon_v - 0.098$	0.	0.02	0.02	0.08	0.08	**0.38**	**0.18**	**0.78**	0.	0.	0.02	0.02
11,12	$\epsilon_v - 0.123$	**0.28**	0.	0.	**0.31**	0.	**0.26**	**0.19**	**0.56**	0.	0.	0.01	0.01
13	$\epsilon_v - 0.140$	0.	**0.21**	0.06	**0.28**	0.	0.12	**0.21**	**0.60**	0.	0.	0.	0.
15,16	$\epsilon_v - 0.175$	0.	0.06	0.01	0.14	0.02	**0.26**	0.05	**0.73**	0.	0.	0.	0.
18	$\epsilon_v - 0.189$	0.	0.04	**0.13**	**0.27**	0.07	**0.16**	0.04	**0.69**	0.	0.	0.	0.
23,24	$\epsilon_v - 0.223$	0.	0.05	0.01	0.14	0.01	**0.33**	**0.12**	**0.69**	0.	0.	0.02	0.02

TABLE VII. Analysis of the significant absorption peaks for a dot with 23.9Å diameter. The peak letters refer to the labelling of the peaks in Figs. 10 and 8. Peak energies are calculated according to Eq.(12). The valence and conduction indices refer to the number of the state from the band edge (i.e. VBM and CBM have index 1 etc). The envelope function information summarizes the results from Table III.

All energies are in eV.

Peak	Peak Energy	Initial valence state				Final conduction state			
		Index	Energy	Envelope	F	Index	Energy	Envelope	F
(a)	1.780	1,2	-6.035	s+p	2.01	1	-3.991	s	1.20
(b)	1.863	3,4	-6.101	p	2.51	1	-3.991	s	1.20
(c)	1.904	5,6	-6.166	$s+p+d$	2.04	1	-3.991	s	1.20
(d)	2.072	12,13	-6.301	$s+d$	3.25	1	-3.991	s	1.20
(e)	2.140	14,15	-6.365	$s+d$	3.75	1	-3.991	s	1.20
(f)	2.220	1,2	-6.035	s	2.13	6,7,8	-3.673	p	2.19
(g)	2.231	3,4	-6.101	p	2.47	6,7,8	-3.673	p	2.19
(h)	2.343	5,6	-6.166	$s+d+f$	2.04	6,7,8	-3.673	p	2.19
(i)	2.410	7,8	-6.202	$p+f$	3.05	6,7,8	-3.673	p	2.19
(j)	2.462	9,10	-6.249	d	3.41	6,7,8	-3.673	p	2.19

TABLE VIII. Analysis of the significant absorption peaks for a dot with 30.3Å diameter. The peak letters refer to the labelling of the peaks in Figs. 10 and 8. Peak energies are calculated according to Eq.(12). The valence and conduction indices refer to the number of the state from the band edge (i.e. VBM and CBM have index 1 etc). The envelope function information summarizes the results from Table IV.
All energies are in eV.

Peak	Peak Energy	Initial valence state				Final conduction state			
		Index	Energy	Envelope	F	Index	Energy	Envelope	F
(a)	1.549	1,2	-5.938	s	1.75	1	-4.232	s	1.27
(b)	1.594	3,4	-5.976	p	1.98	1	-4.232	s	1.27
(c)	1.676	5,6	-6.064	$s+p+d$	1.99	1	-4.232	s	1.27
(d)	1.757	12,13	-6.134	$s+d$	2.57	1	-4.232	s	1.27
(e)	1.826	15	-6.200	$s+d$	3.03	1	-4.232	s	1.27
(f)	1.996	1,2	-5.938	$s+p$	1.77	6,7,8	-3.787	p	2.15
(g)	2.041	3,4	-5.976	p	1.98	6,7,8	-3.787	p	2.15
(h)	2.143	7,8	-6.076	$s+d+f$	2.72	6,7,8	-3.787	p	2.15
(i)	2.202	12,13	-6.134	$s+d$	2.57	6,7,8	-3.787	p	2.15
(j)	2.281	17,18	-6.208	$d+f$	3.03	6,7,8	-3.787	p	2.15
(k)	2.335	23,24	-6.270	p	3.24	6,7,8	-3.787	p	2.15

TABLE IX. Analysis of the significant absorption peaks for a dot with 36.9Å diameter. The peak letters refer to the labelling of the peaks in Figs. 10 and 8. Peak energies are calculated according to Eq.(12). The valence and conduction indices refer to the number of the state from the band edge (i.e. VBM and CBM have index 1 etc). The envelope function information summarizes the results from Table V.

All energies are in eV.

Peak	Peak Energy	Initial valence state				Final conduction state			
		Index	Energy	Envelope	F	Index	Energy	Envelope	F
(a)	1.374	1,2	-5.872	s	1.75	1	-4.374	s	1.12
(b)	1.401	3,4	-5.895	p	1.92	1	-4.374	s	1.12
(c)	1.508	5,6	-5.989	$s+p+d$	2.18	1	-4.374	s	1.12
(d)	1.533	11,12	-6.023	$s+d$	2.48	1	-4.374	s	1.12
(e)	1.610	15	-6.098	$s+d+g$	3.14	1	-4.374	s	1.12
(g)	1.803	3,4	-5.895	p	1.93	2,3,4	-3.982	p	1.81
(h)	1.901	5,6	-5.989	$p+d+f$	2.76	2,3,4	-3.982	p	1.81
(i)	2.942	12,13	-6.023	$s+d$	2.73	2,3,4	-3.982	p	1.81
(j)	2.020	16,17	-6.106	f	3.16	2,3,4	-3.982	p	1.81
(k)	2.061	23,24	-6.144	p	3.20	2,3,4	-3.982	p	1.81

TABLE X. Analysis of the significant absorption peaks for a dot with 42.2Å diameter. The peak letters refer to the labelling of the peaks in Figs. 10 and 8. Peak energies are calculated according to Eq.(12). The valence and conduction indices refer to the number of the state from the band edge (i.e. VBM and CBM have index 1 etc). The envelope function information summarizes the results from Table VI.

All energies are in eV.

Peak	Peak Energy	Initial valence state				Final conduction state			
		Index	Energy	Envelope	F	Index	Energy	Envelope	F
(a)	1.209	1,2	-5.8260	$s+p$	1.77	1	-4.516	s	1.11
(c)	1.335	11,12	-5.9491	$p+d$	2.48	1	-4.516	s	1.11
(g)	1.588	3,4	-5.8401	p	1.90	2,3,4	-4.156	p	1.92
(h)	1.675	7,8	-5.9240	$s+p+f$	2.66	2,3,4	-4.156	p	1.92
(i)	1.717	13	-5.9660	$p+d+f$	2.93	2,3,4	-4.156	p	1.92
(j)	1.760	15,16	-6.0087	$p+f$	3.07	2,3,4	-4.156	p	1.92
(k)	1.800	23,24	-6.0491	p	3.19	2,3,4	-4.156	p	1.92

TABLE XI. Comparison of the current multi-band pseudopotential assignment and the k.p assignment from Ref. [11] of the experimentally observed optical transitions in Ref. [11]. The initial states and final states of each transition are denoted by nQ_F, where n is the principal quantum number, Q the lowest angular momentum component of the wavefunction and F total angular momentum. Note, it is only possible to determine the envelope function angular momentum and total angular momentum for the multi-band pseudopotential wavefunctions.

Peak	Pseudopotential assignment	Closest Expt. Peak from Ref. [11]	k.p assignment from Ref. [11]
(a)	$S_{3/2} \rightarrow S_{1/2}$	E_1	$2S_{3/2} \rightarrow 1S_{1/2}$
(b)	$P_{5/2} \rightarrow S_{1/2}$	Not observed	No prediction
(c)	$P_{5/2} \rightarrow S_{1/2}$	E_2/E_3	No prediction
(d)	$S_{5/2} \rightarrow S_{1/2}$	E_2	No prediction
(e)	$S_{7/2} \rightarrow S_{1/2}$	E_3	$2S_{3/2} \rightarrow 1S_{1/2}$
(g) and (h)	$P_{5/2} \rightarrow P_{3/2}$	E_5	$1P_{3/2} \rightarrow 1P_{3/2}$ $1P_{3/2} \rightarrow 1P_{1/2}$
(j)	$S_{7/2} \rightarrow P_{3/2}$	E_6	$2S_{1/2} \rightarrow 1S_{1/2}$
(k)	$P_{7/2} \rightarrow P_{3/2}$	E_7	$1P_{1/2} \rightarrow 1P_{3/2}$ $1P_{1/2} \rightarrow 1P_{1/2}$