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Excited States and Valley Effects in a Negatively Charged Donor in a Si FinFET

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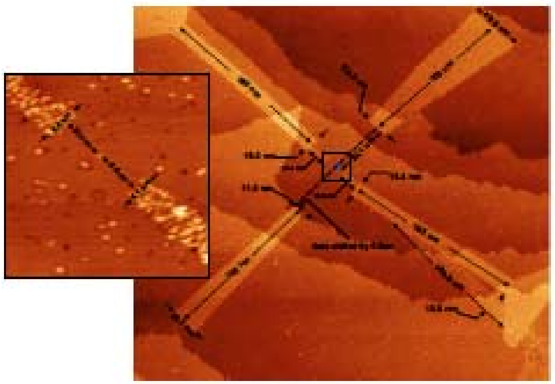
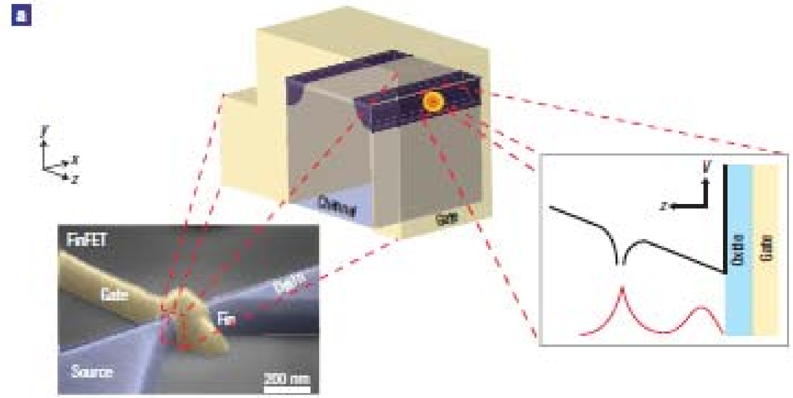
Single impurity devices in Si

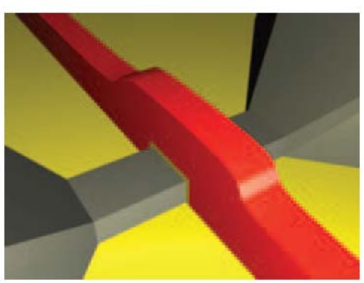
- Top-down vs. Bottom-up
- Unintentional doping vs. controlled dopant implantation

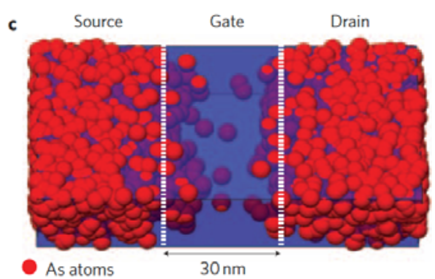


Simmons group, (unpublished work) (2010)

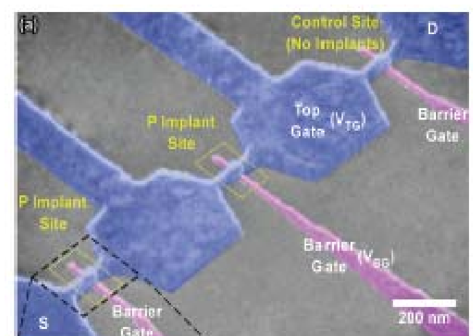


Rogge group, Nature Physics 4, 656 (2008)





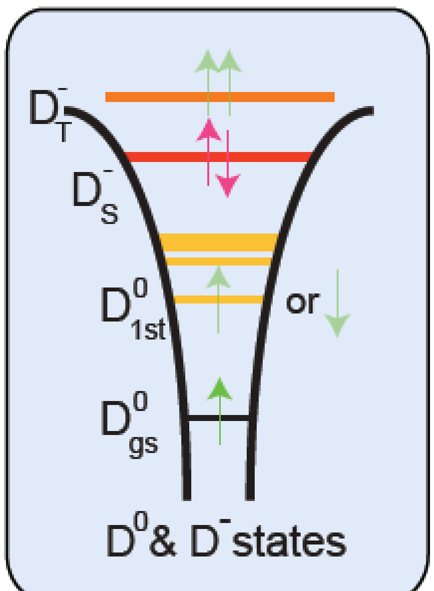
Sanquer group,
Nature Nanotechnology 5, 133 (2010)

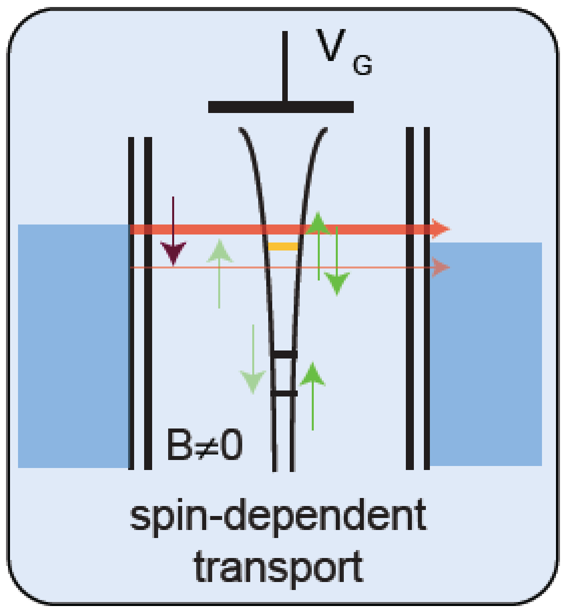


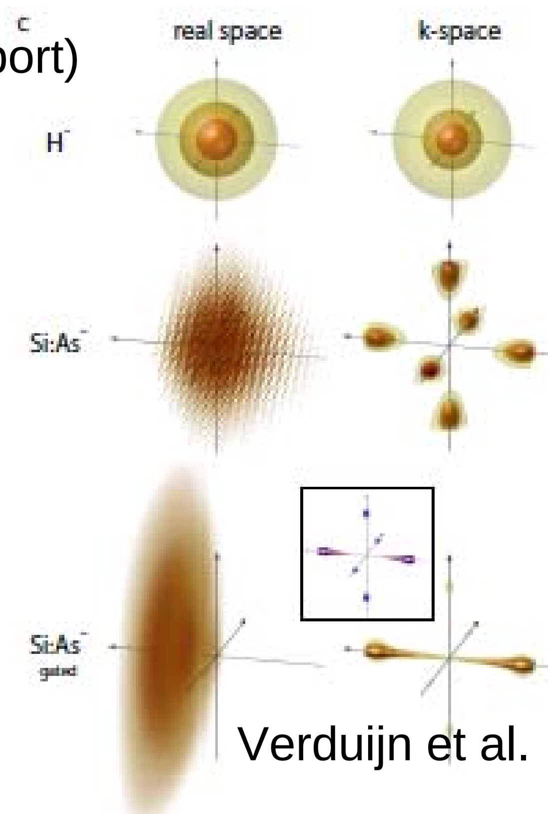
Dzurak group, Nano Lett. 10(1),11 (2010)

Why D- is important?

- 2e atomic system in silicon matrix (hydrogenic ion)
- pure atomic states (different from QD states)
- lab for studying momentum space contributions to few electron atomic physics
- known valley-orbit splitting
- Spin dependent tunneling for spin measurement
- Spin dependent relaxation (Lifetime enhanced transport)



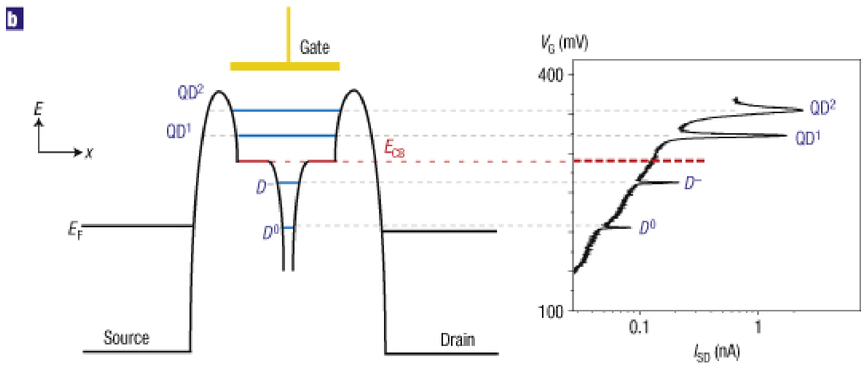


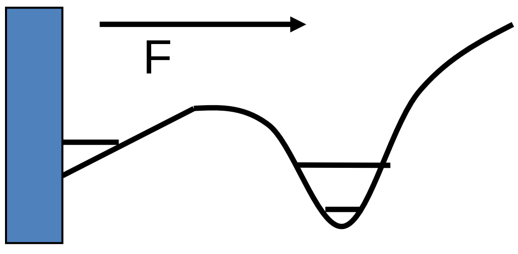


Verduijn et al.

Outline of results

Experiment: Transport spectroscopy in donor-interface well
Theory: Atomistic tight binding + SCF Hartree Fock (over 1M atoms)





Barrier-Si-impurity

Previously known facts about D-:

• Bulk measurements show only 1 bound singlet.

• P donor D- at -1.7 meV, As D- at -2 meV (bulk case).

Results from this work:

1. Quantum confinement affects charging energy
2. Excited bound D- states observed including triplets at large E-fields
3. Valley dependence of exchange
4. Lifetime Enhanced Transport

Lansbergen, Rahman, Verduijn, Klimeck, Hollenberg, Rogge, arXiv 1008.1381 (2010)

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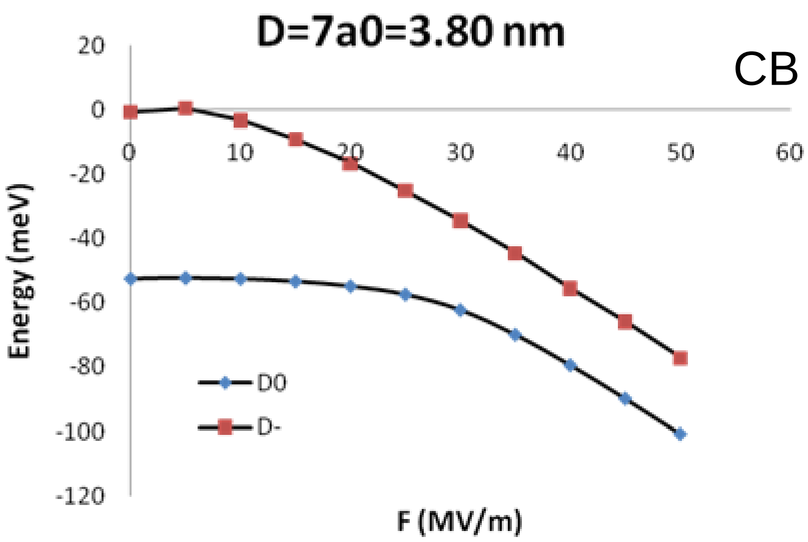
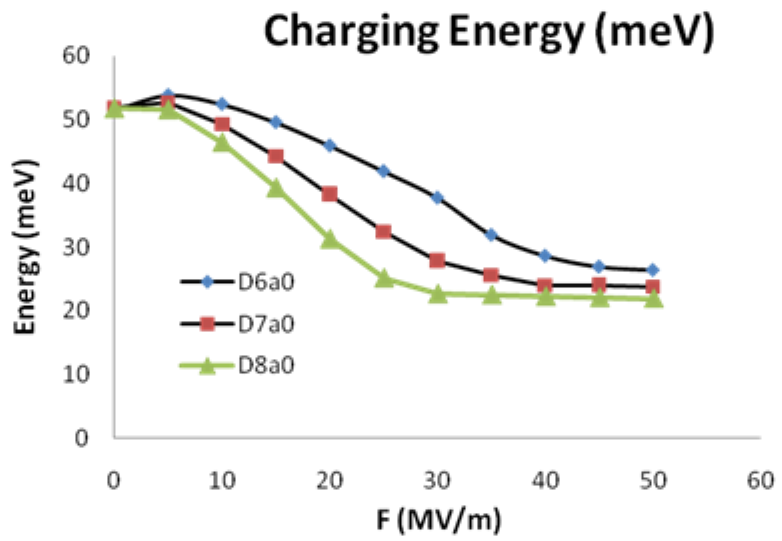
D- charging energy from SCF TB





- Bulk P charging energy (CE) from SCF TB: 42.4 meV
- Known value from optical measurements: 43.9 meV

- CE depends on wf localization between interface well and donor well

- Other factors: Corner confinement, dielectric mismatch

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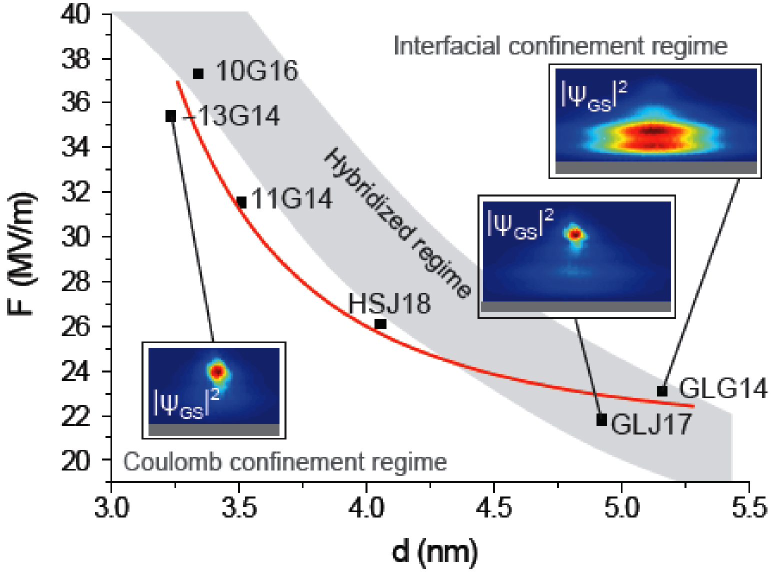
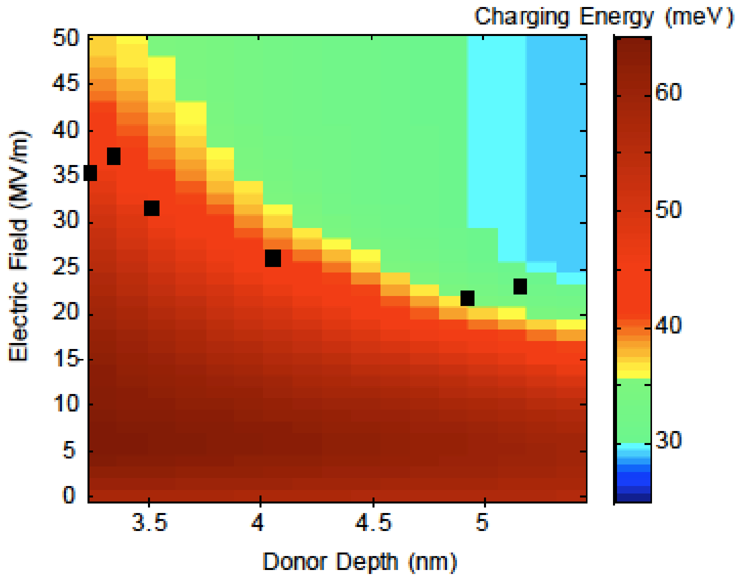
D- charging energy (TB vs experiment)

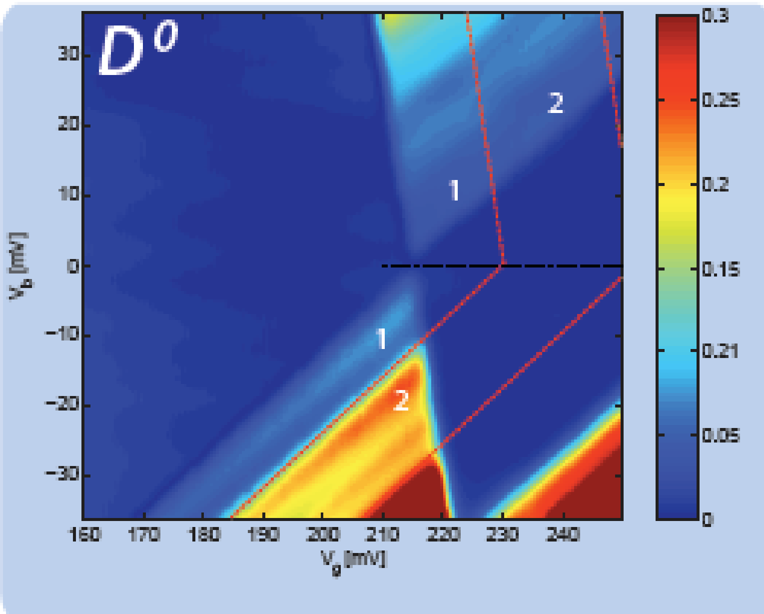


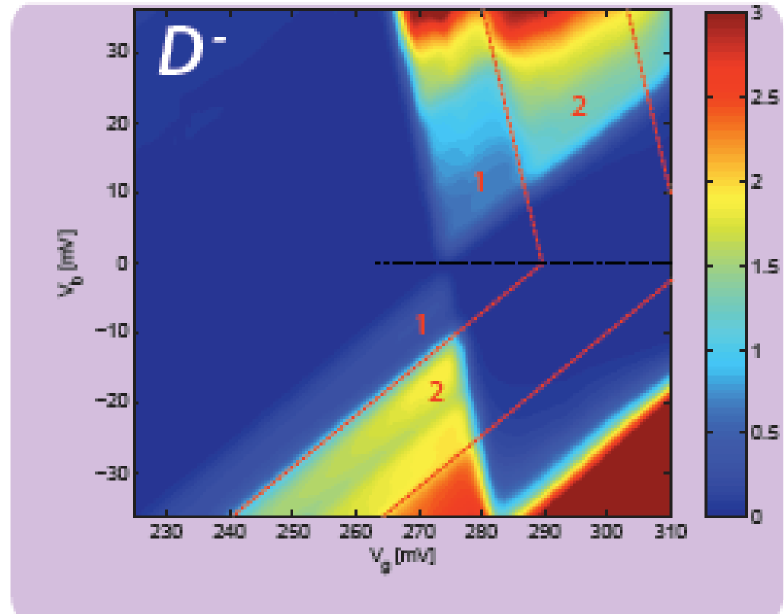


- Donor depths and fields known for 6 devices (previous work on D0 excited state spectroscopy)
- CE calculated for the same devices and compared to measurements
- Agreement within 5 meV, expected trends
- Sources of error: 1.5 meV accuracy, dielectric screening

Lansbergen, Rahman, Klimeck, Hollenberg, Rogge, Nature Physics 4, 656 (2008)

Bound excited states of D-





Bound excited D- states observed for the first time.

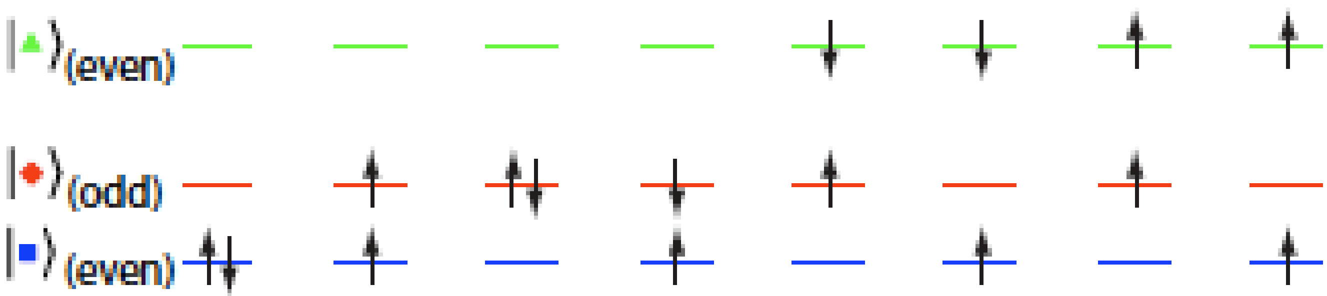
Excited manifold has triplet states also.

Theoretical prediction of D- excited states

b

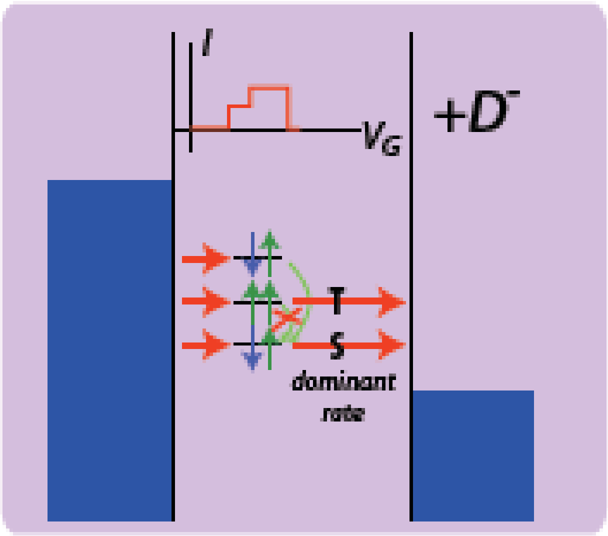
lower manifold wave function	ΔE [meV] theo.	ΔE [meV] exp.	higher manifold wave function	ΔE [meV] theo.	ΔE [meV] exp.
$[\|$■$\rangle\|$■$\rangle\|S\rangle$	0	0	$[\|$▲$\rangle\|$◆$\rangle + \|$◆$\rangle\|$▲$\rangle]\|S\rangle$	7.9	
$[\|$◆$\rangle\|$■$\rangle - \|$■$\rangle\|$◆$\rangle]\|T\rangle$	1.5		$[\|$▲$\rangle\|$■$\rangle + \|$■$\rangle\|$▲$\rangle]\|S\rangle$	8.0	7.5
$[\|$◆$\rangle\|$■$\rangle + \|$■$\rangle\|$◆$\rangle]\|S\rangle$	1.6	1.0	$[\|$▲$\rangle\|$◆$\rangle - \|$◆$\rangle\|$▲$\rangle]\|T\rangle$	8.1	
$[\|$◆$\rangle\|$◆$\rangle\|S\rangle$	1.7		$[\|$▲$\rangle\|$■$\rangle - \|$■$\rangle\|$▲$\rangle]\|T\rangle$	11.2	10-15

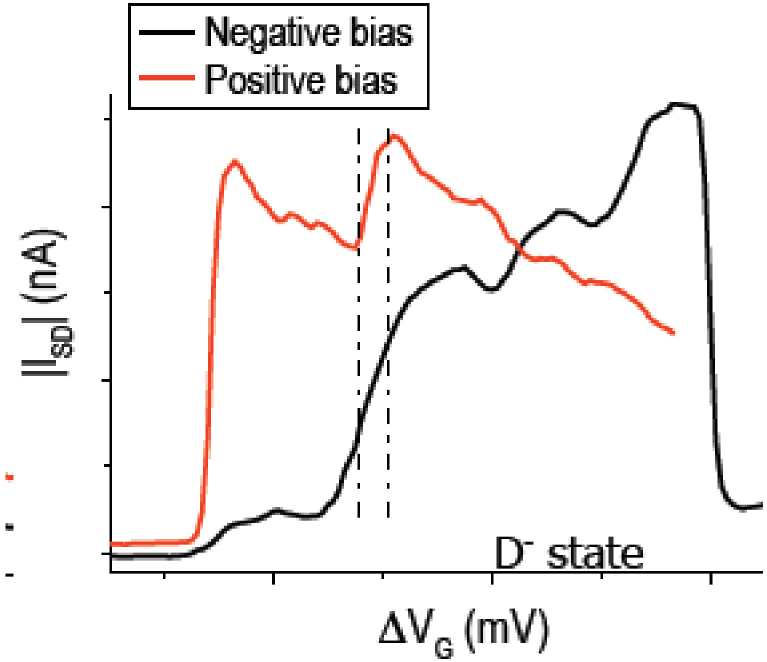
c



Electronic configurations across orthogonal valley states result in small exchange splitting

Lifetime enhanced transport in D-





- in the slow unloading direction only the ground state should be visible (asym. 1/2000)
- one of the states (steep step) in the excited manifold does not relax
- stronger coupling of this states leads to current step
- stronger coupling without LET can not lead to this step

Conclusions

- Quantitative description of the D- charging energy for 6 device samples
- Observation of bound D- excited states for the first time
- Qualitative agreement of excited state energies and spin symmetries
- Vanishing exchange splitting in the orthogonal valley states
- Observation of lifetime enhanced transport through D- excited states