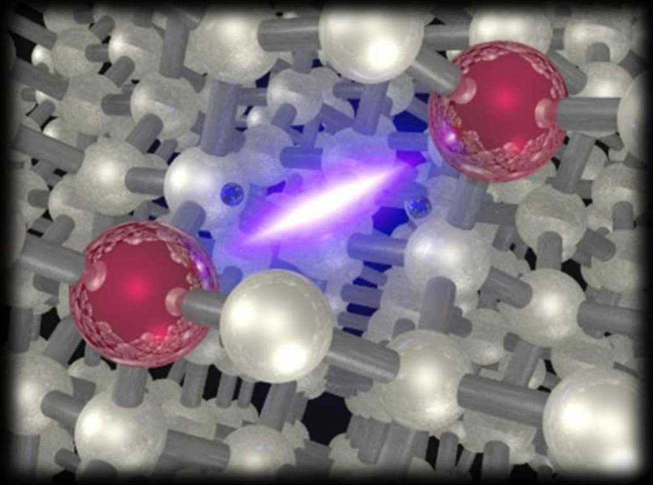
SAND2020-2632C

Full configuration interaction simulations of exchange coupled donors in silicon in an effective mass theory framework



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QUANTUM COMPUTATION COMMUNICATION TECHNOLOGY

UNSW SYDNEY

Australian Government

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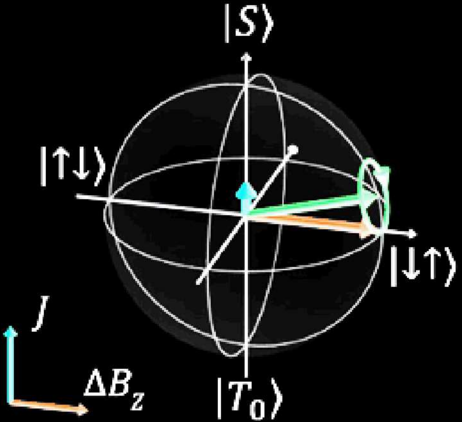
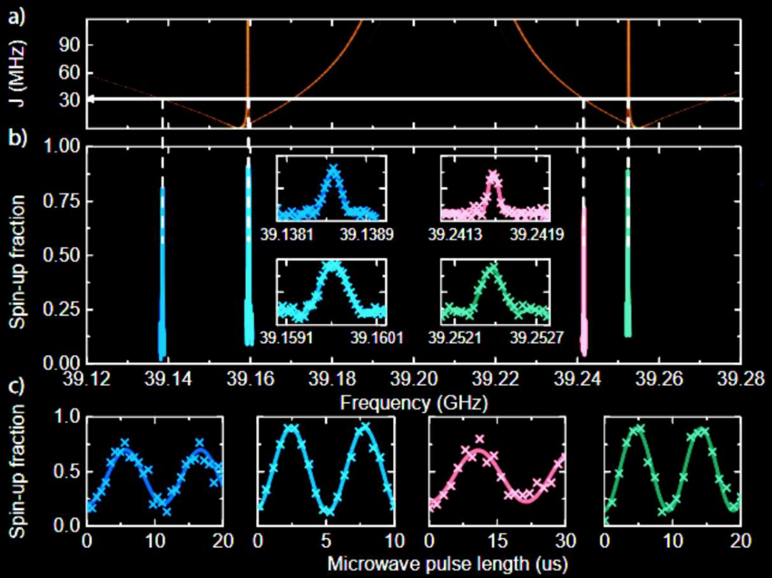
Two-Qubit Gates in Silicon

1. Weak exchange and ESR pulses



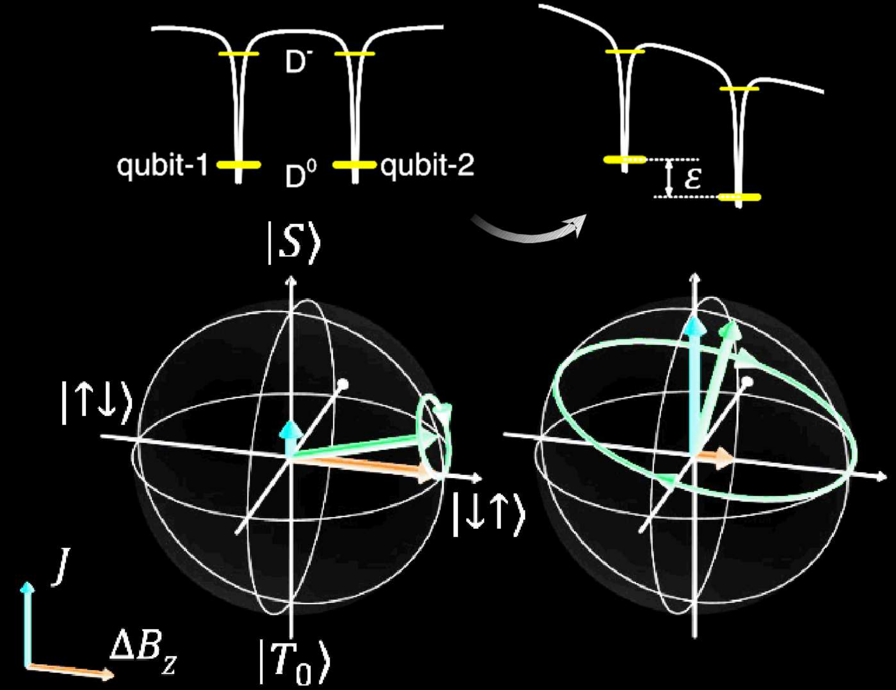
Donors



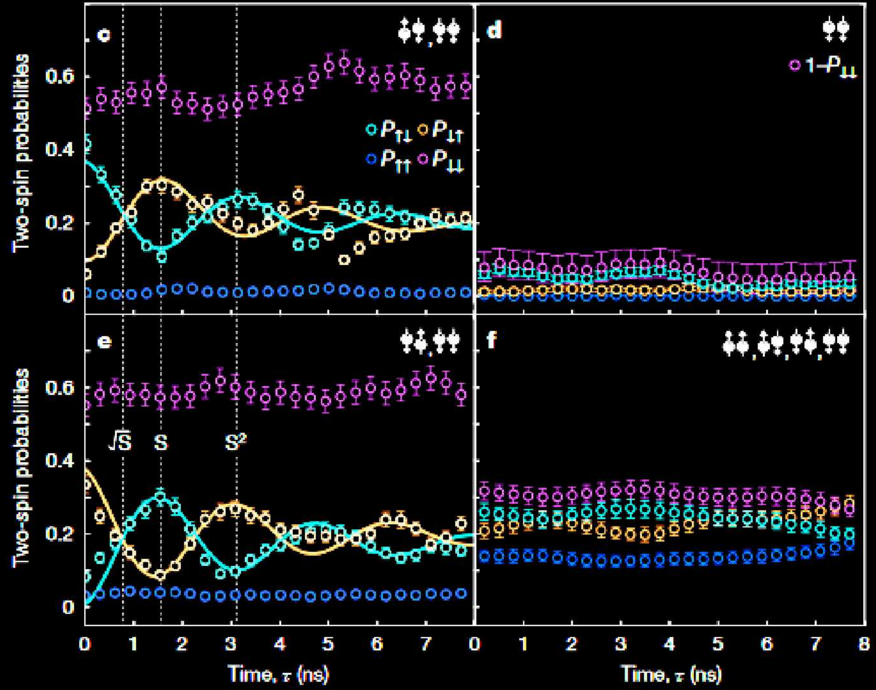
Madzik M., et al. in preparation

Two-Qubit Gates in Silicon

2. Strongly tuneable exchange



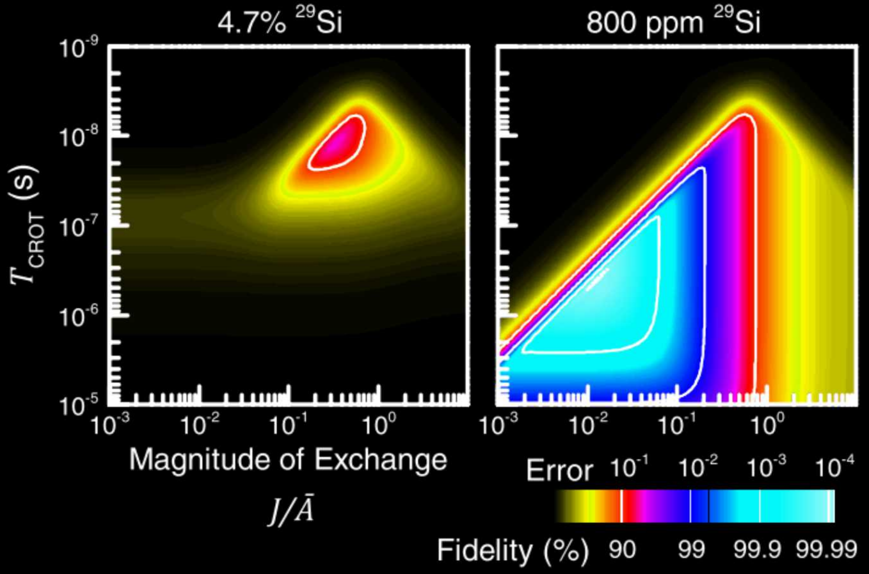
SWAP oscillations:



He Y. et al. *Nature* 571.7765 (2019): 371-375.

Requirements for High Fidelity

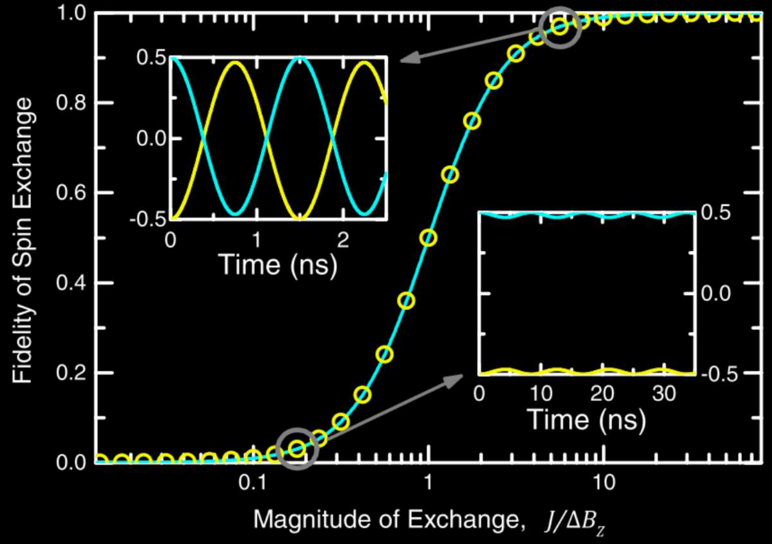
1. Weak exchange and ESR pulses



$$J < \frac{A}{10} = 11.7\ \mathrm{MHz}$$

Kalra R. et al. *Physical Review X* 4.2 (2014): 021044.

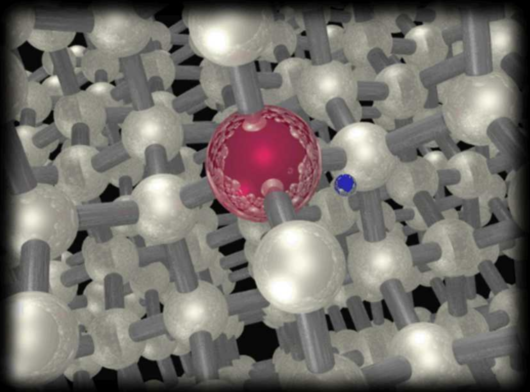
2. Strongly tuneable exchange



For high Fidelity:

$J \sim 10\mathrm{MHz}$ ⟺ Tuneable ⟺ $J \sim 1\mathrm{GHz}$

Multivalley Effective Mass Theory



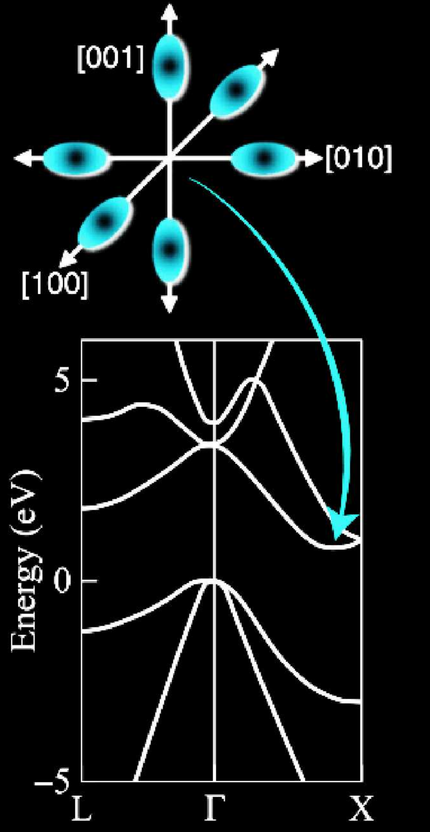
Ansatz:

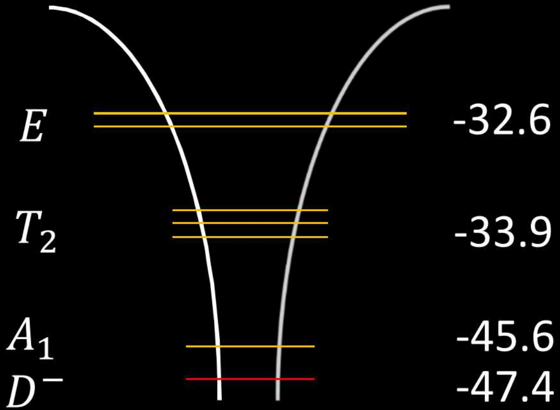
$$\psi(\vec{r}) = \sum_{j=1}^{6} F_j(\vec{r})\phi_j(\vec{r})$$

Ingredients:

- Effective donor potential
  $$U(\vec{r}) \propto 1/r$$
- Anisotropic effective mass
  $$m_{\parallel} \quad m_{\perp}$$
- Valley orbit coupling
  $$V_{i,j}^{VO}(\vec{r}) = \langle \phi_i | U(\vec{r}) | \phi_j \rangle$$

Gamble J.K. et al. *Physical Review B* 91.23 (2015): 235318.



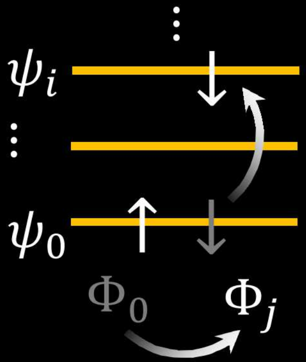


Configuration Interaction

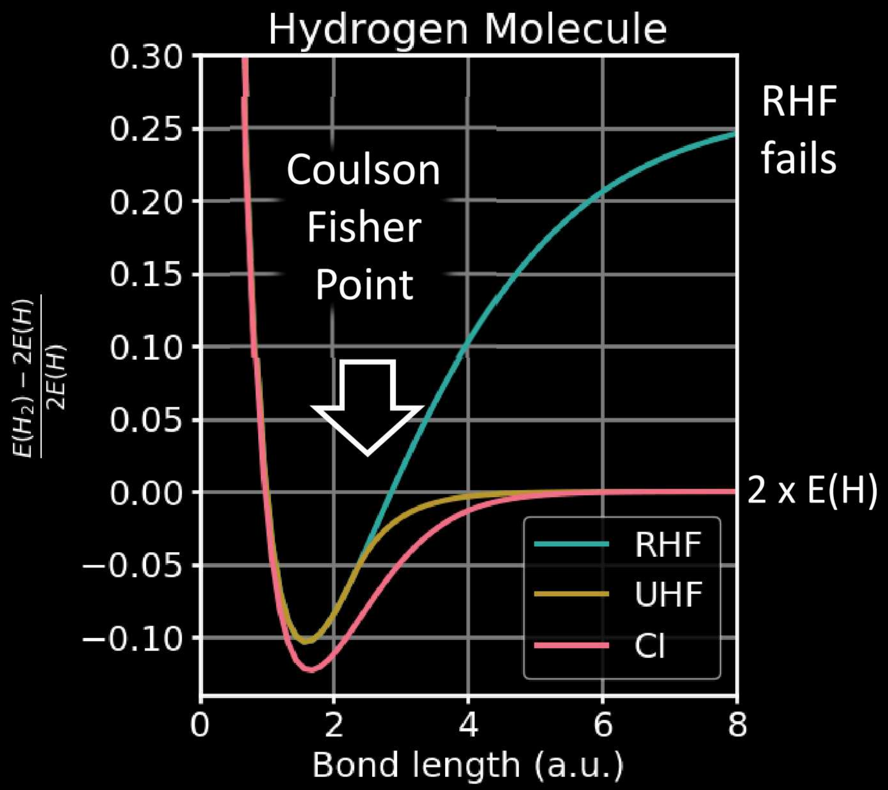
Hartree-Fock Approximation:

$$\Phi = \frac{1}{\sqrt{2}}\left(|\psi_i\psi_j\rangle|\uparrow\downarrow\rangle - |\psi_j\psi_i\rangle|\downarrow\uparrow\rangle\right)$$

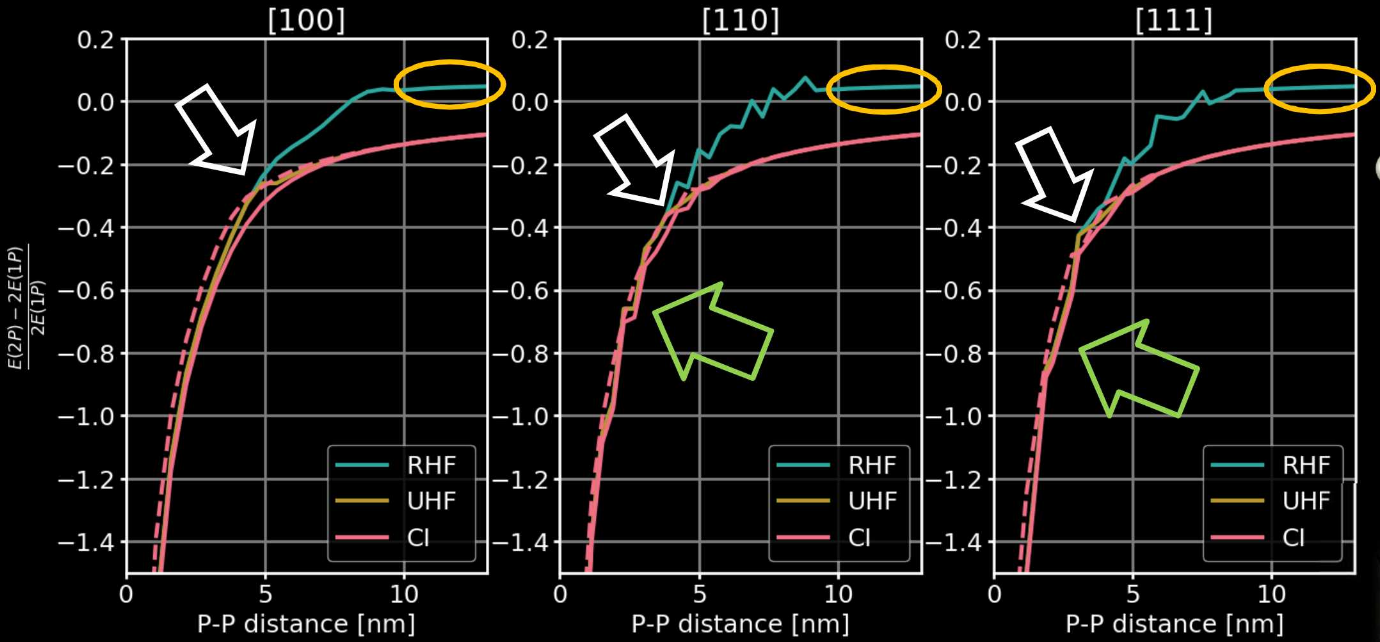
Configuration Interaction:



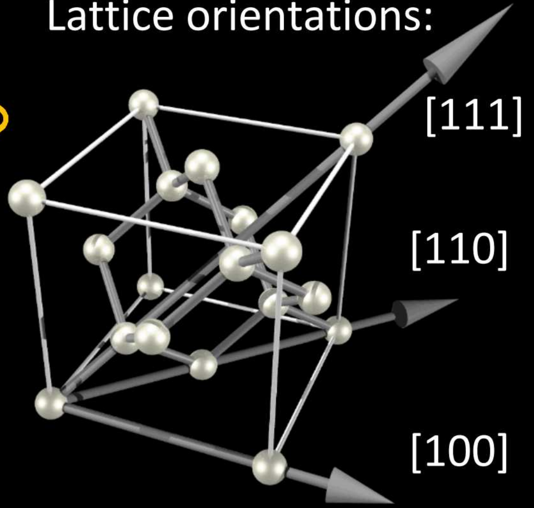
$$\Psi = \sum_i a_i \Phi_i$$

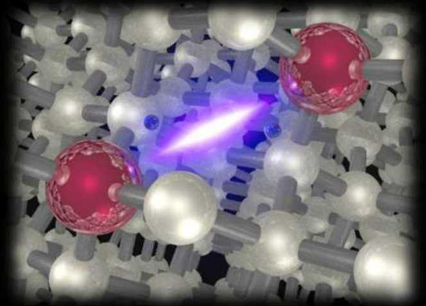


Phosphorus Donor Molecule



Lattice orientations:

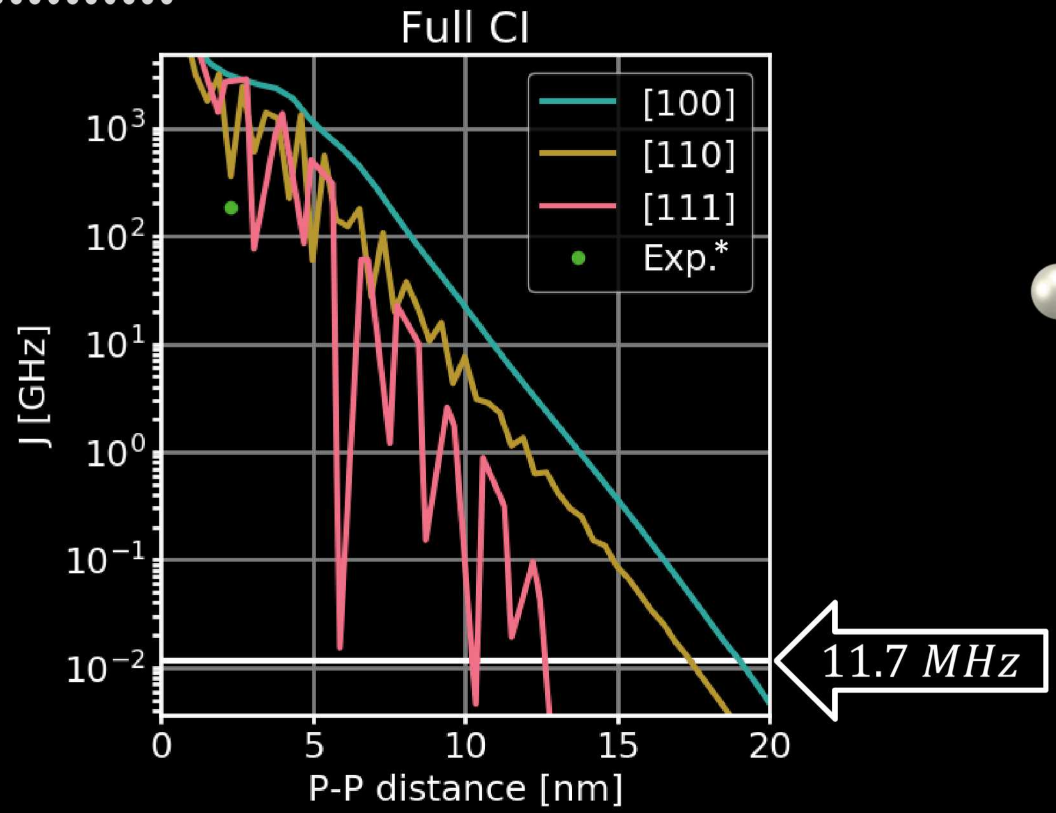




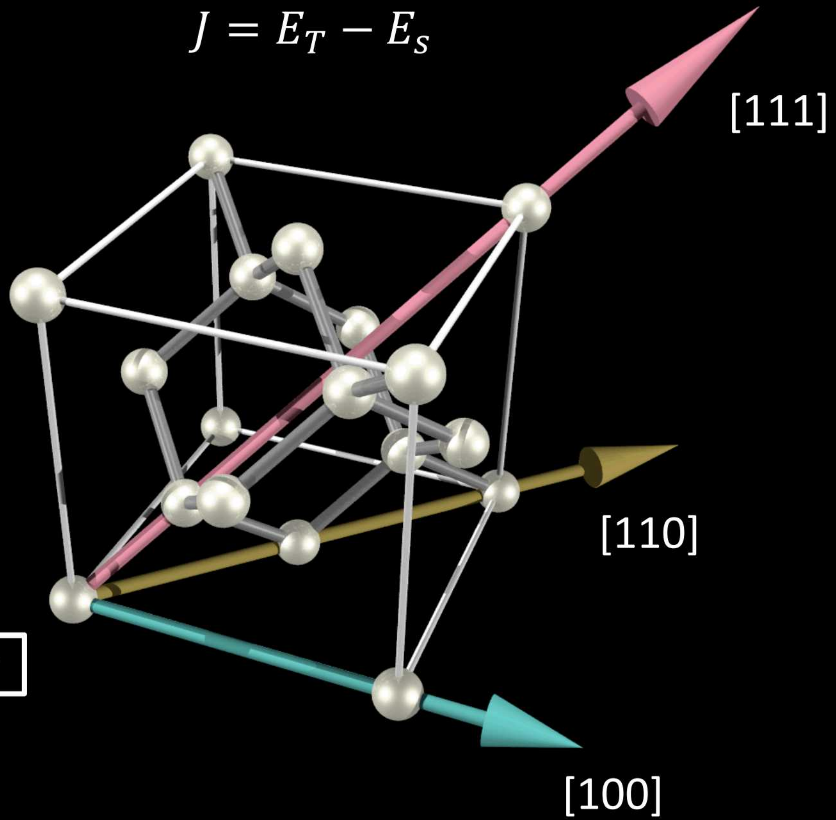
RHF fails for large distances

Valley oscillations along [110] and [111]

Exchange Interaction

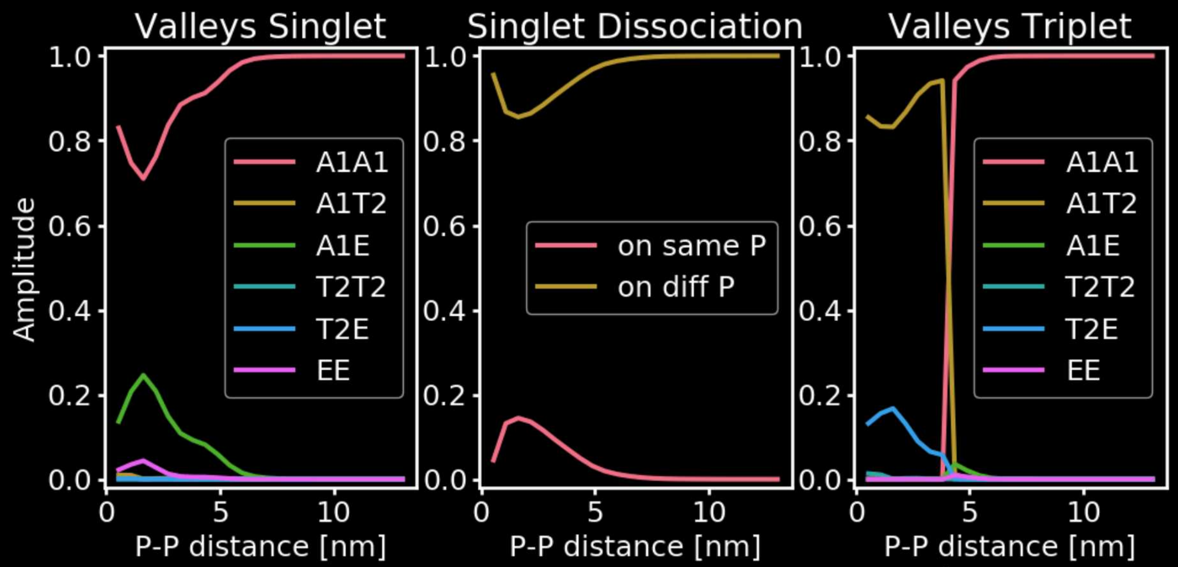


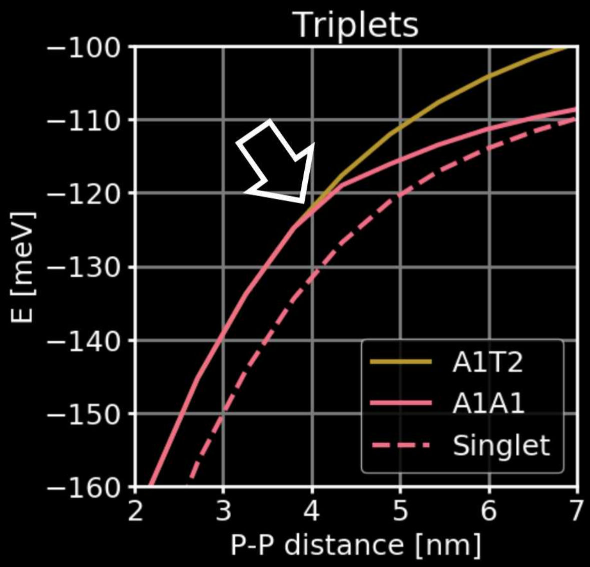
$J = E_T - E_S$

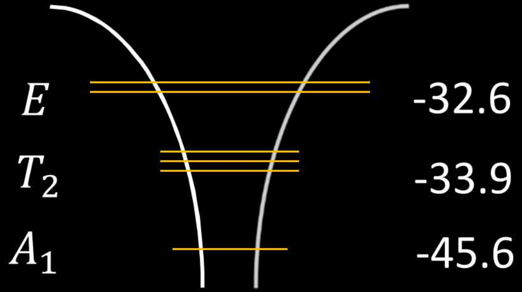


*González-Zalba et al. *Nano letters* 14.10 (2014): 5672-5676

Valley Configuration [100]



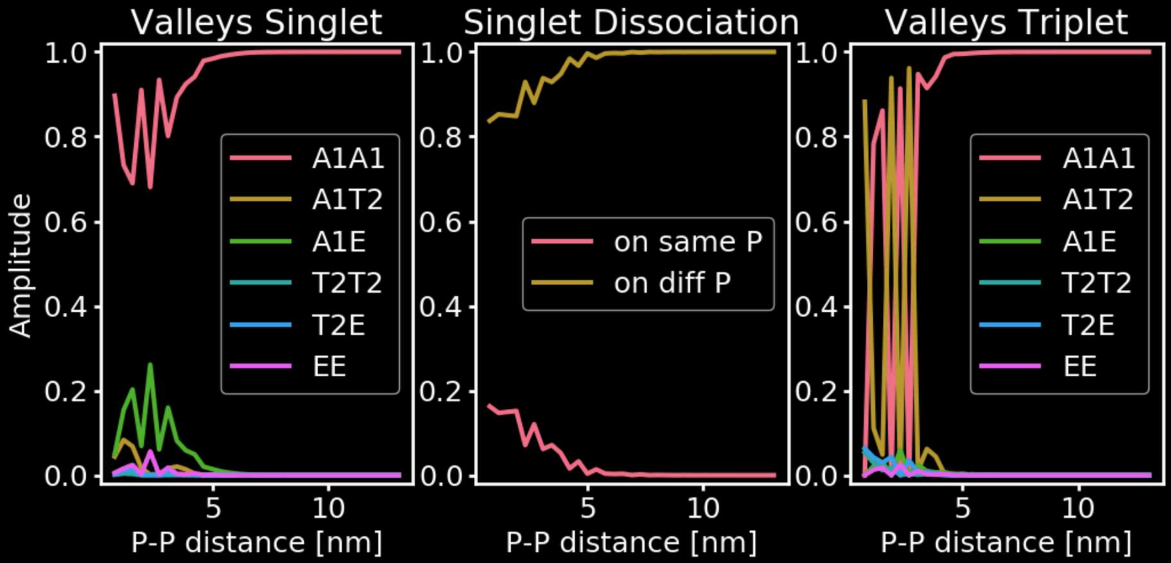




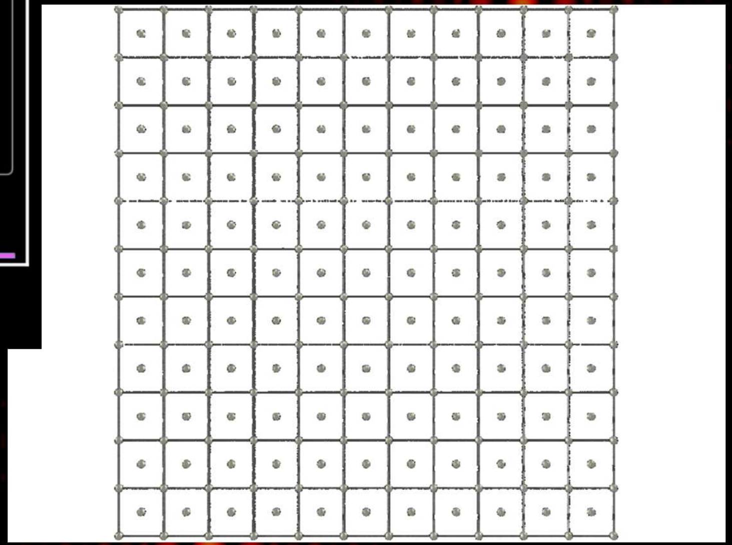
Anticrossing with first excited triplet.

Dehollain, Juan P., et al. *Physical review letters* 112.23 (2014): 236801.

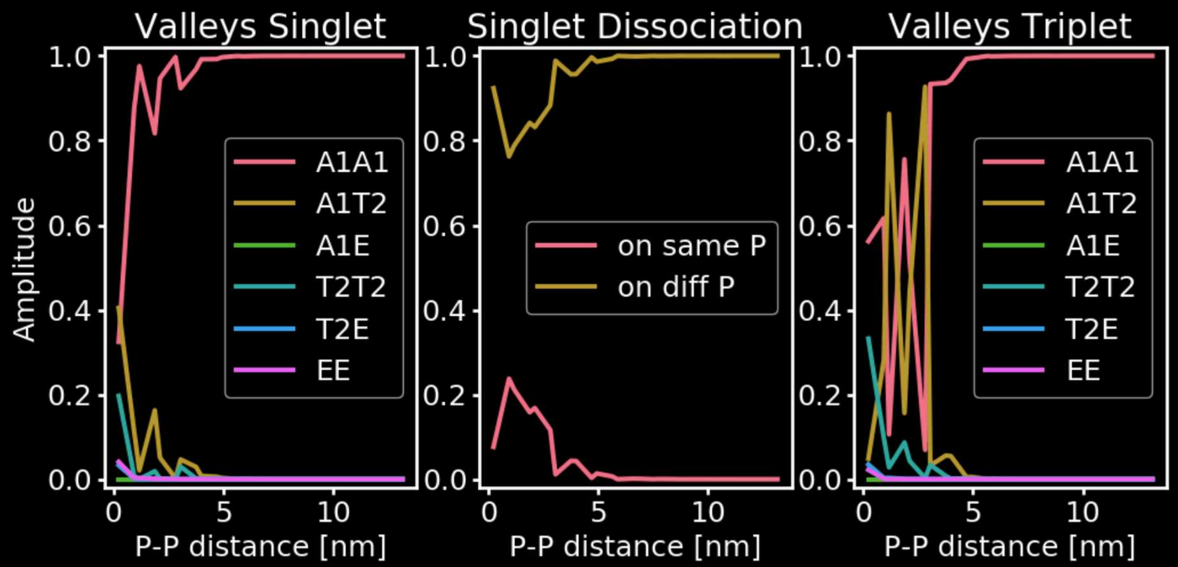
Valley Oscillations along [110]

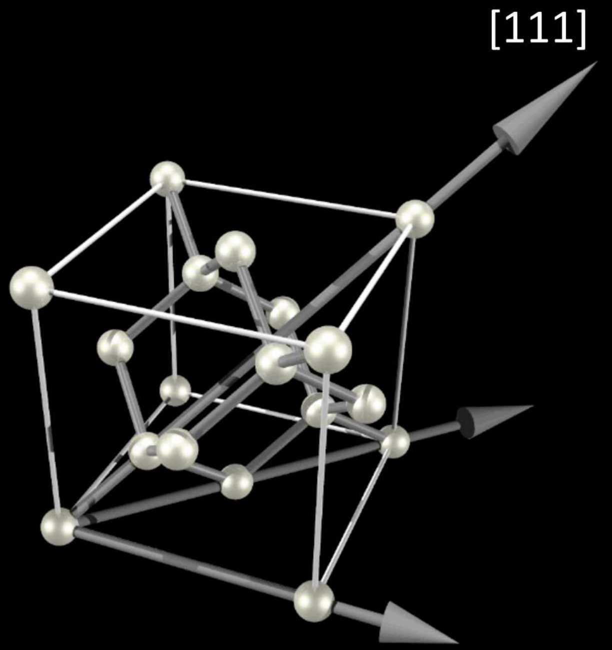


Strength of state overlap oscillates

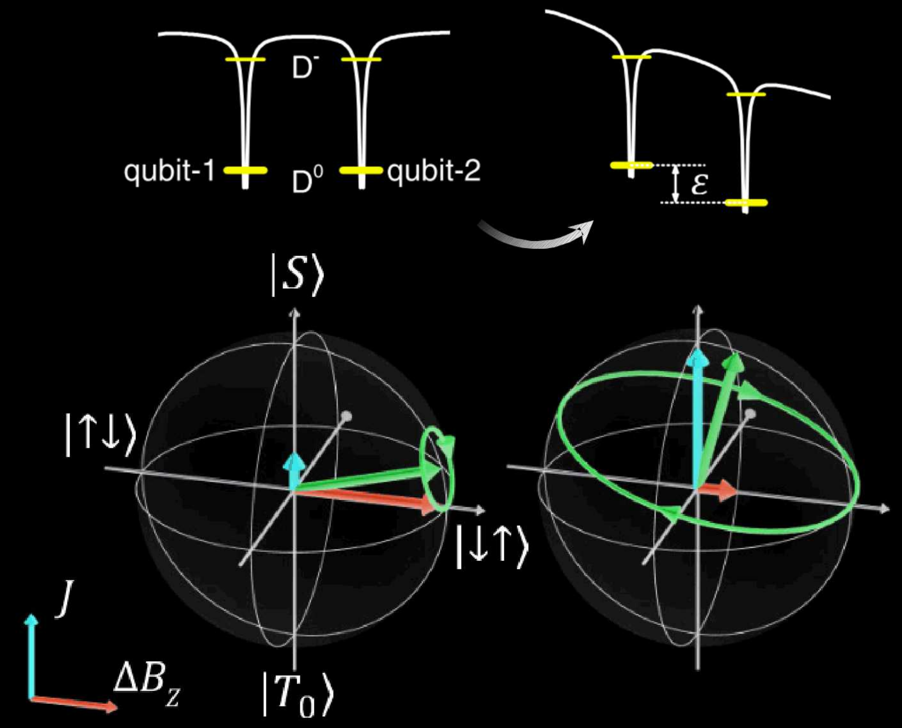


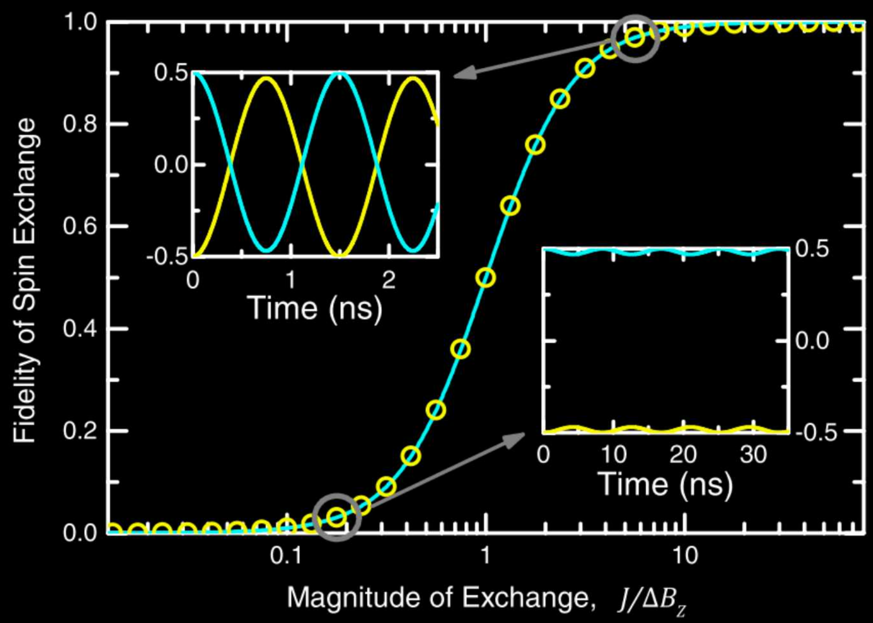
Valley Oscillations along [111]





Electric Tunability for SWAP Gates



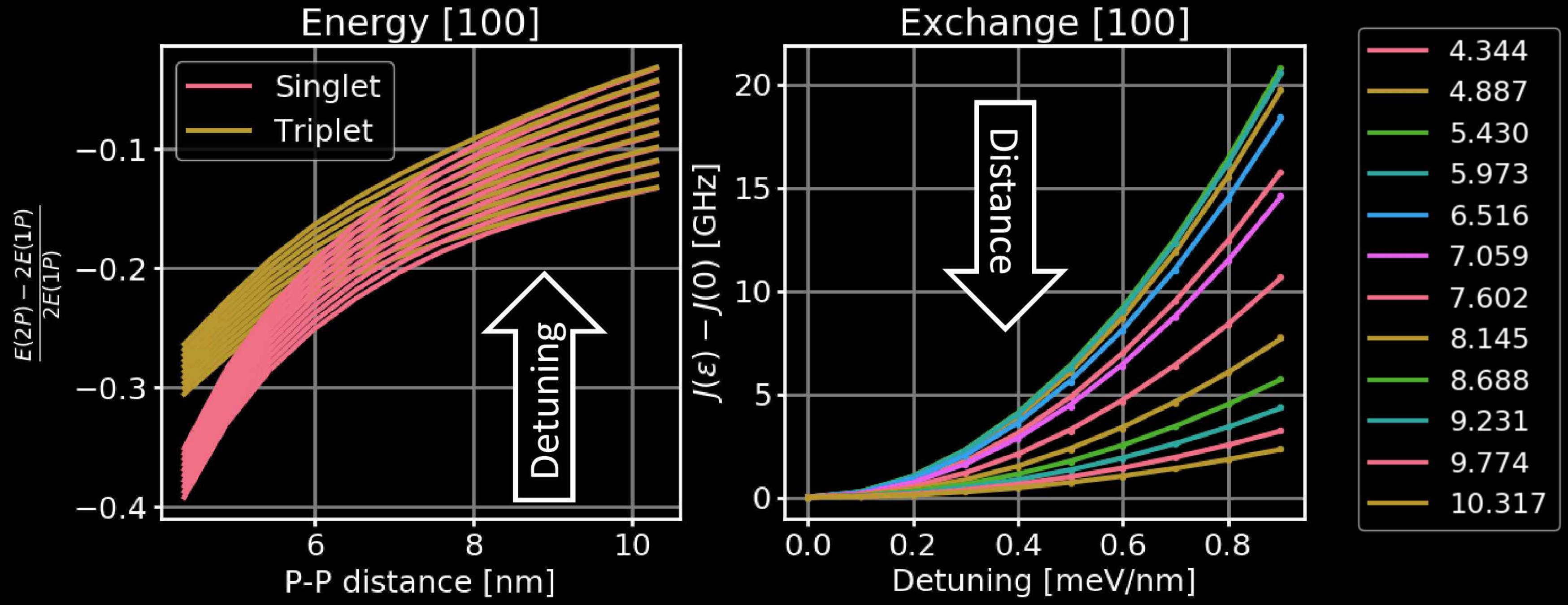


For high Fidelity:

$J \sim 10\mathrm{MHz}$ ⟺ Tuneable ⟺ $J \sim 1\mathrm{GHz}$

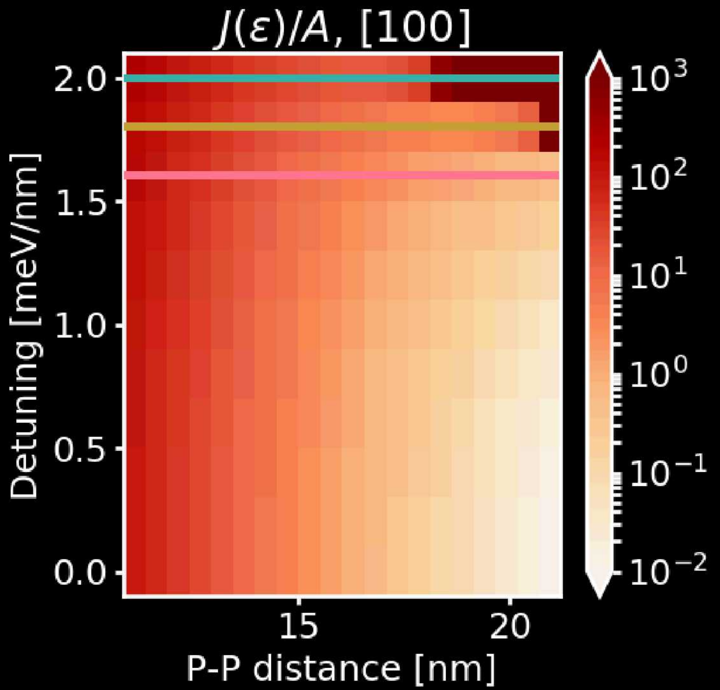
Kalra R. et al. *Physical Review X* 4.2 (2014): 021044.

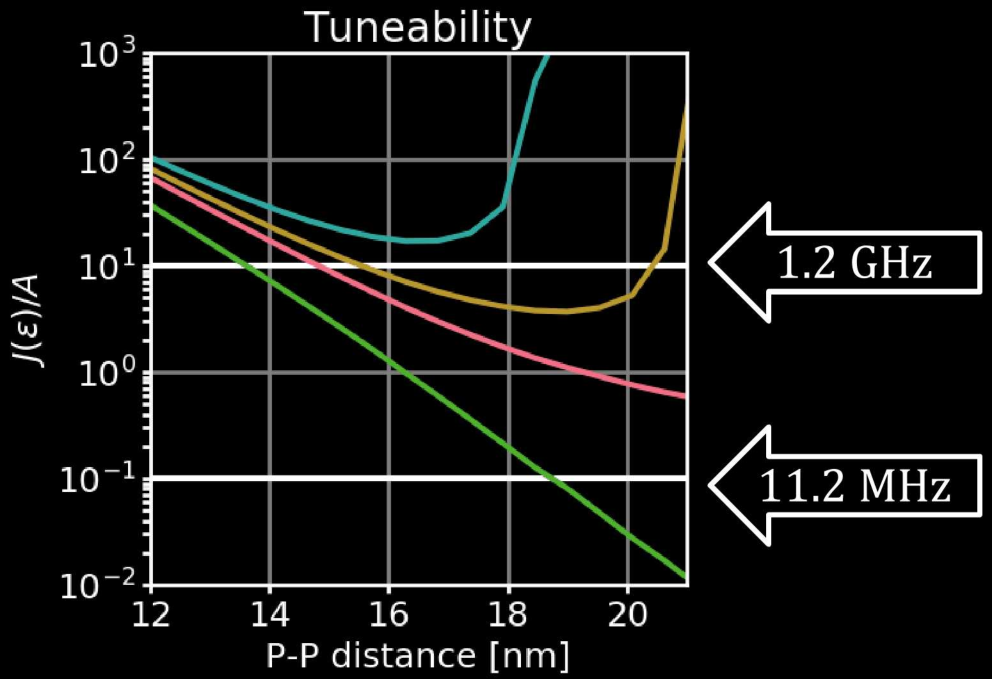
Exchange Tunability



Quadratic growth

Implementing a SWAP Gate



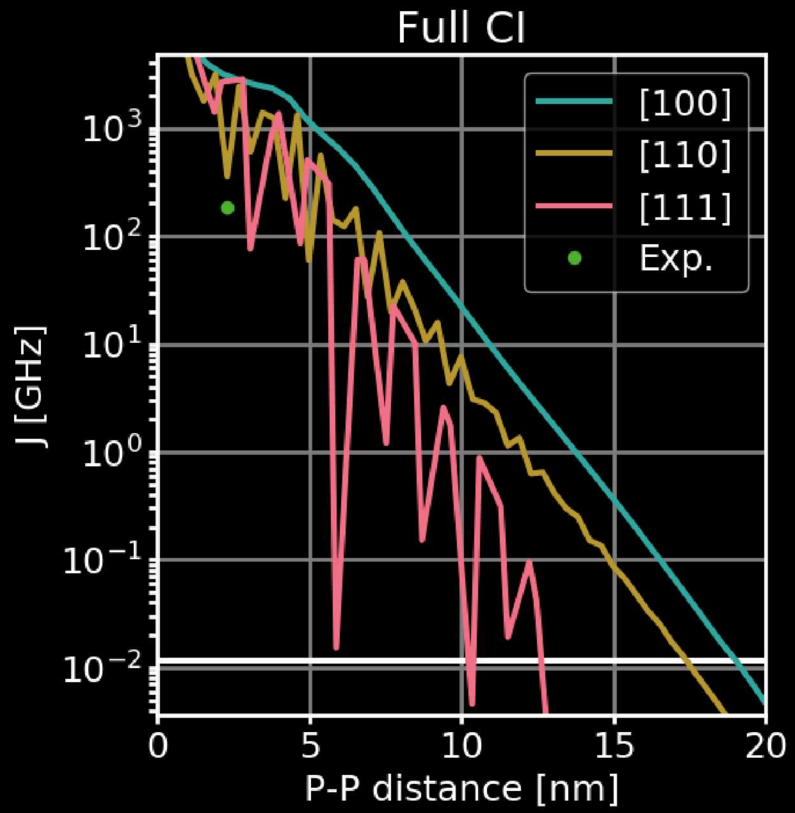


Tunability:

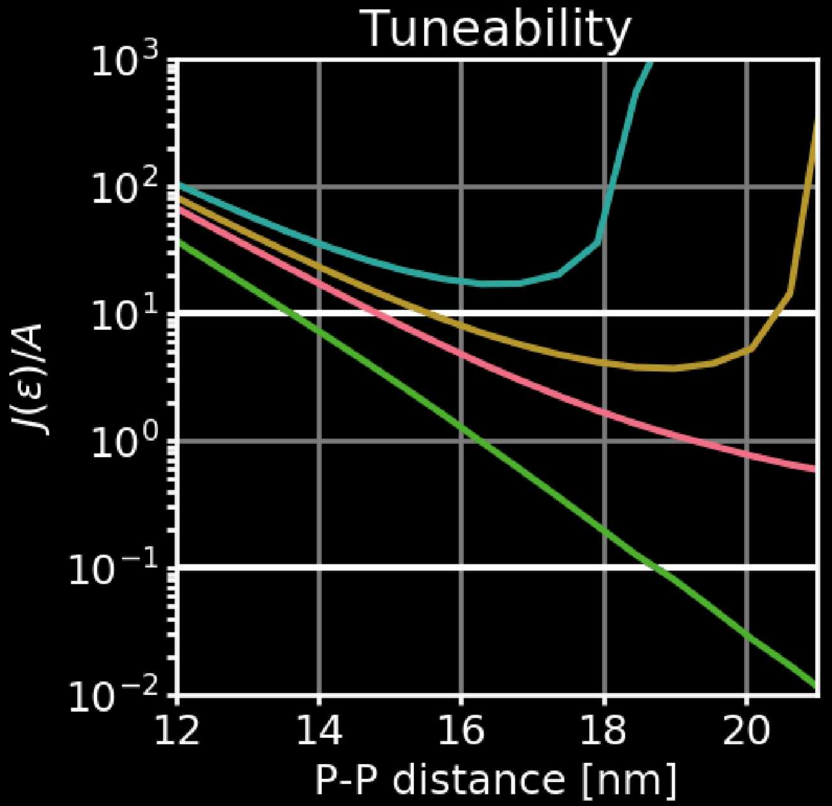
$$d_{[100]} = 20.63\ \mathrm{nm}$$
$$\Delta\varepsilon = 1.8\ \mathrm{meV/nm}$$

1.9 MHz 1.7 GHz

Highlights



Full CI
[100]
[110]
[111]
Exp.
J [GHz]
P-P distance [nm]



Tuneability
$J(\varepsilon)/A$
P-P distance [nm]