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

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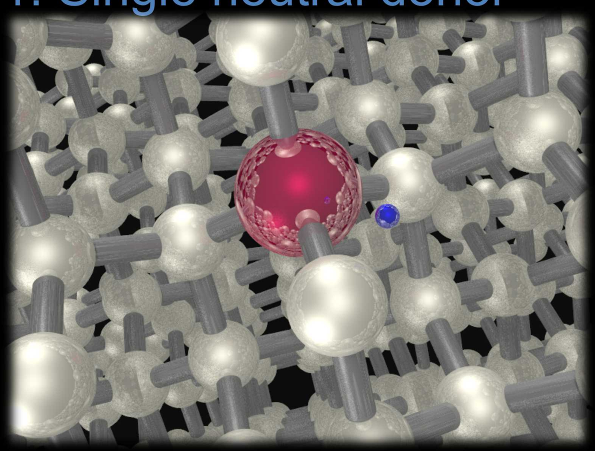
Abstract

Multi-qubit quantum logic gates are the final step to demonstrate the the viability of donor spin qubits in silicon for quantum computation applications. Proposed two-qubit gates rely on the electron-electron exchange interaction which is highly sensitive to the relative placements of the donors in the silicon lattice[1]. For two proximal phosphorus donors an inversion of the hierarchy of the valley-orbital split states has been observed, i.e. the crossing of the bonding combination of T2 states below that of the antibonding A1[2]. Here, we use a full configuration interaction method within an established multivalley effective mass theory framework[3] to model the two-electron wavefunction for different donor configurations. Specifically, we investigate the exchange interaction and valley population along different lattice orientations.

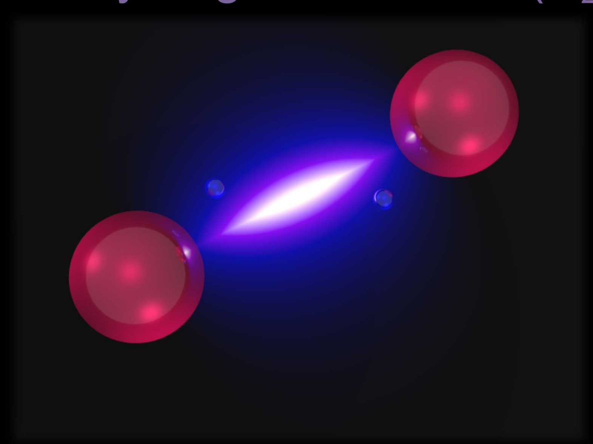
[1] R. Kalra, Phys. Rev. X **4(2)**, 021044 (2014) [2] J.P. Dehollain, Phys. Rev. Lett. **112(23)**, 236801 (2014) [3] J.K. Gamble, Phys. Rev. B **91(23)**, 235318 (2015)

Introduction

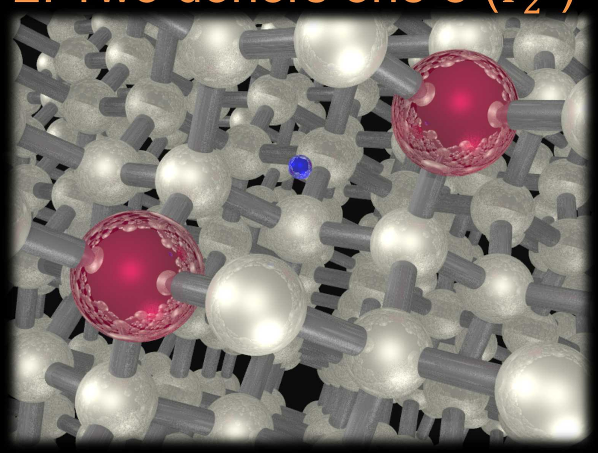
1. Single neutral donor



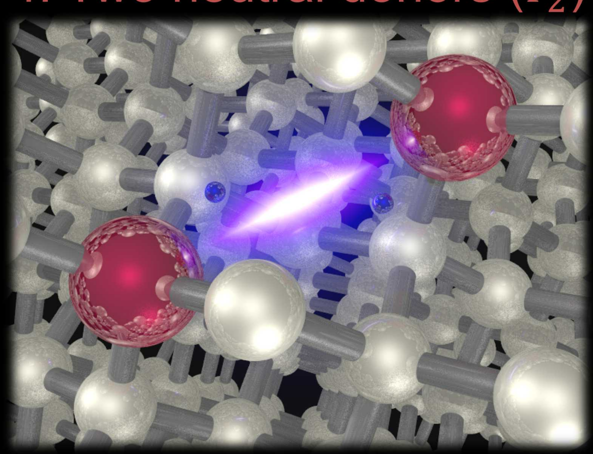
3. Hydrogen Molecule (H_2)



2. Two donors one e (P_2^+)



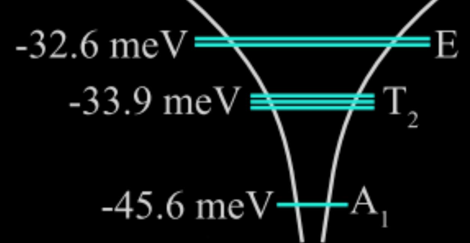
4. Two neutral donors (P_2)

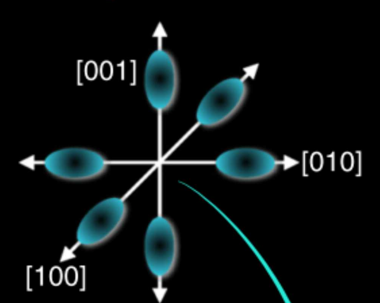


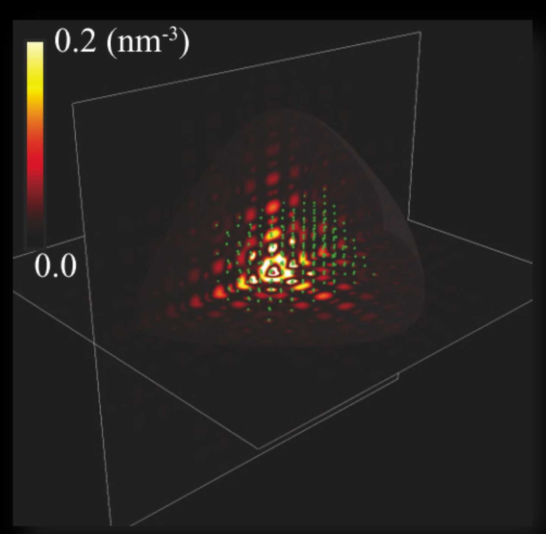
1. Mulitvalley Effective Mass Theory

Ansatz:

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



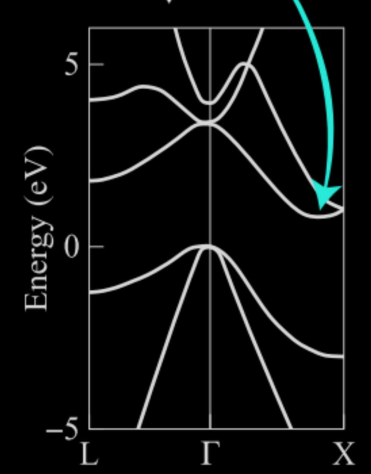




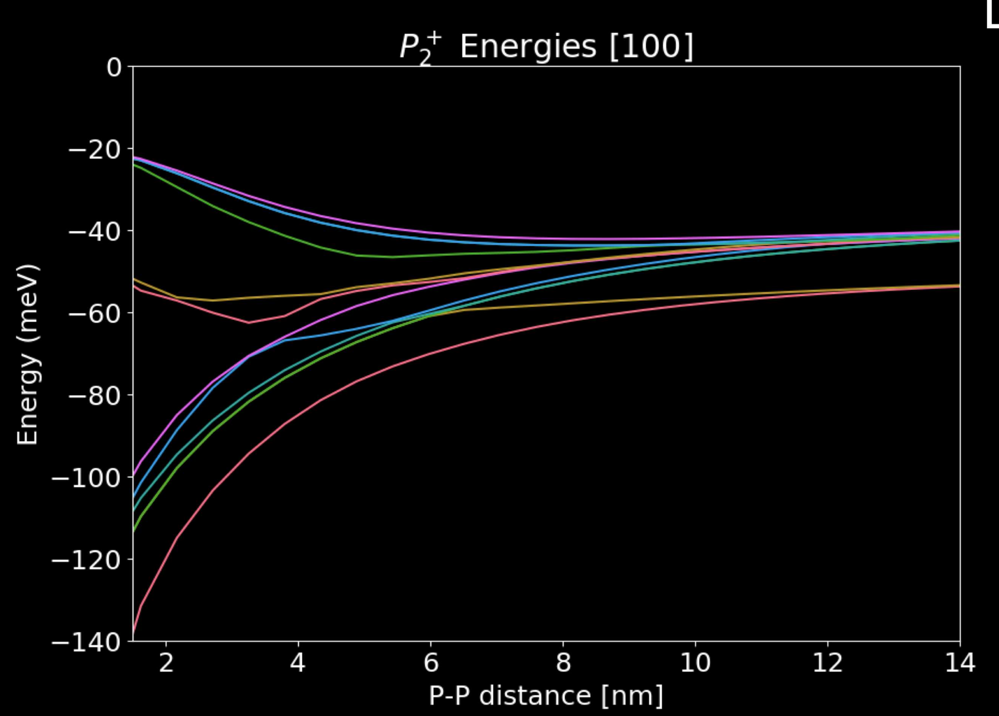
Valley orbit coupling

$$V_{i,j}^{VO}(\vec{r}) = \langle\phi_i|U(\vec{r})|\phi_j\rangle$$

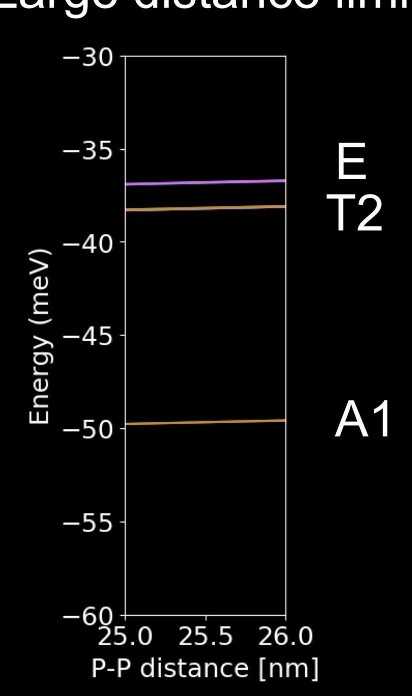
causes the valley splitting

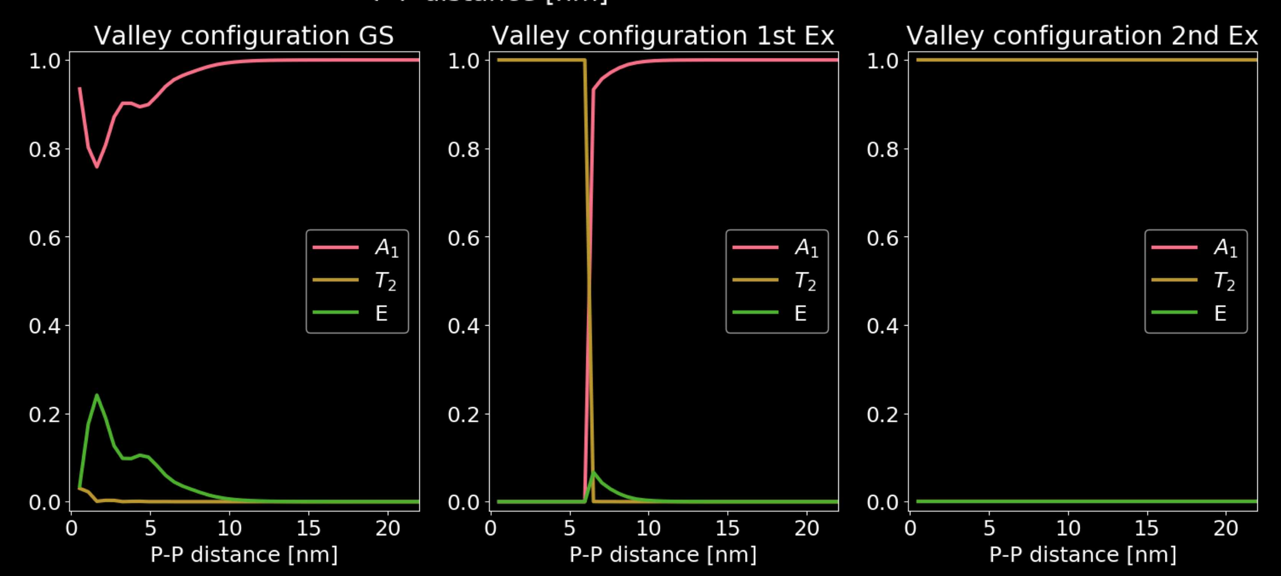


2. P_2^+ Donor Cluster



Large distance limit





3. Hartree-Fock and Configuration Interaction

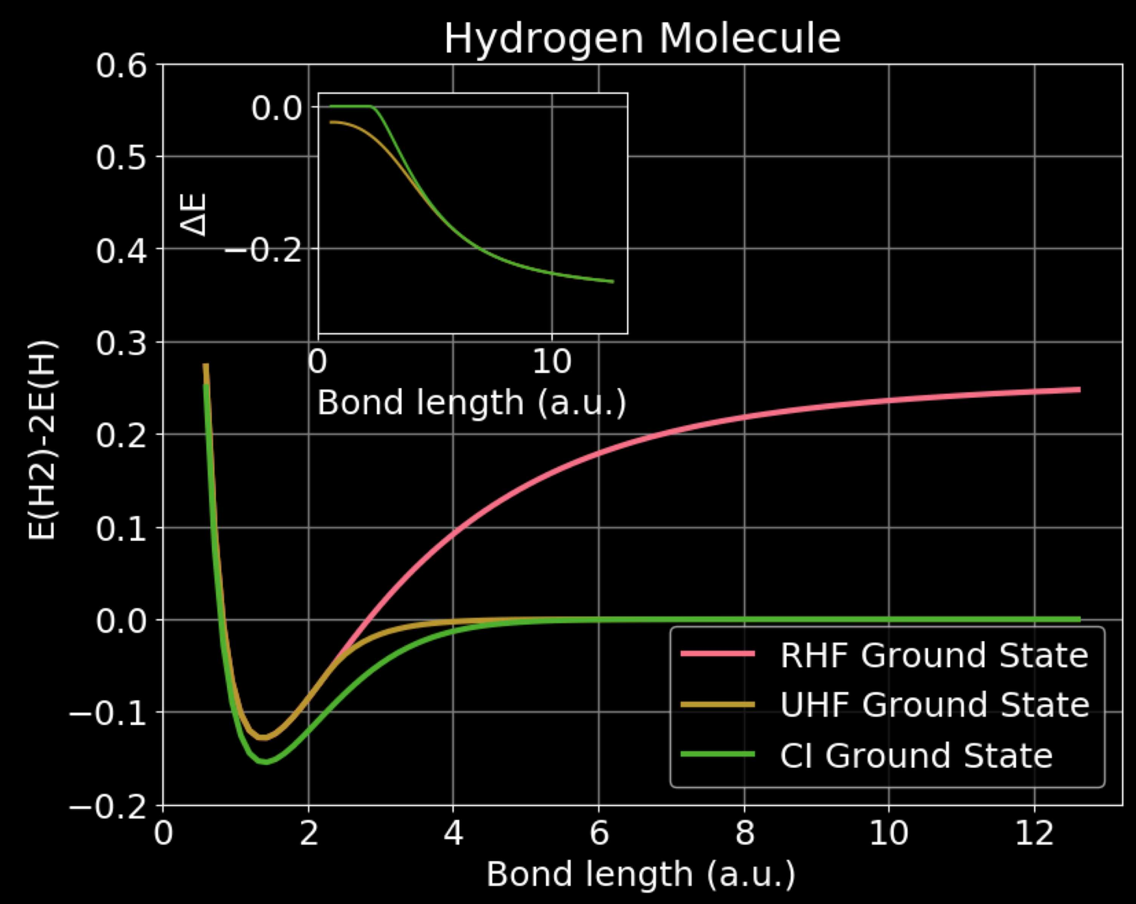
The Hartree-Fock Approximation:

$$\Phi = \frac{1}{\sqrt{2}}(|\psi_i\psi_j\rangle|\alpha\beta\rangle - |\psi_j\psi_i\rangle|\beta\alpha\rangle)$$

Energy of a SD — Fock Operator

$$E = \langle\Phi|H|\Phi\rangle \qquad F_i\psi_i = \varepsilon_i\psi_i$$

minimize

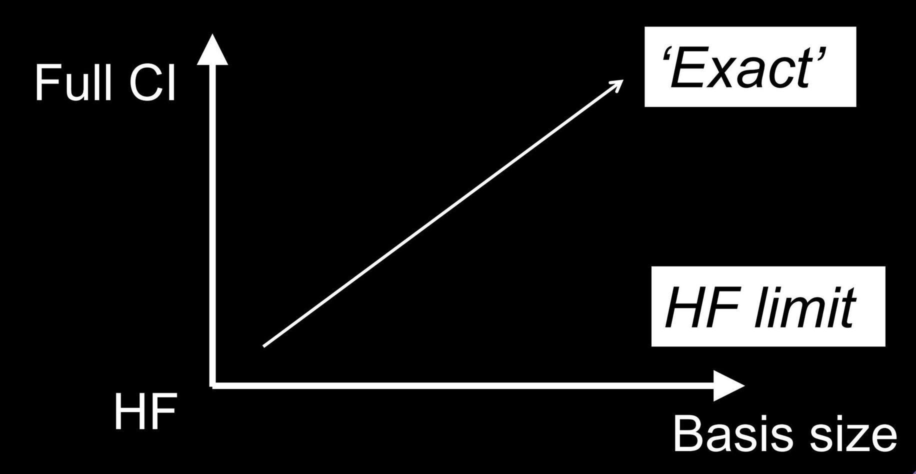


Configuration Interaction:

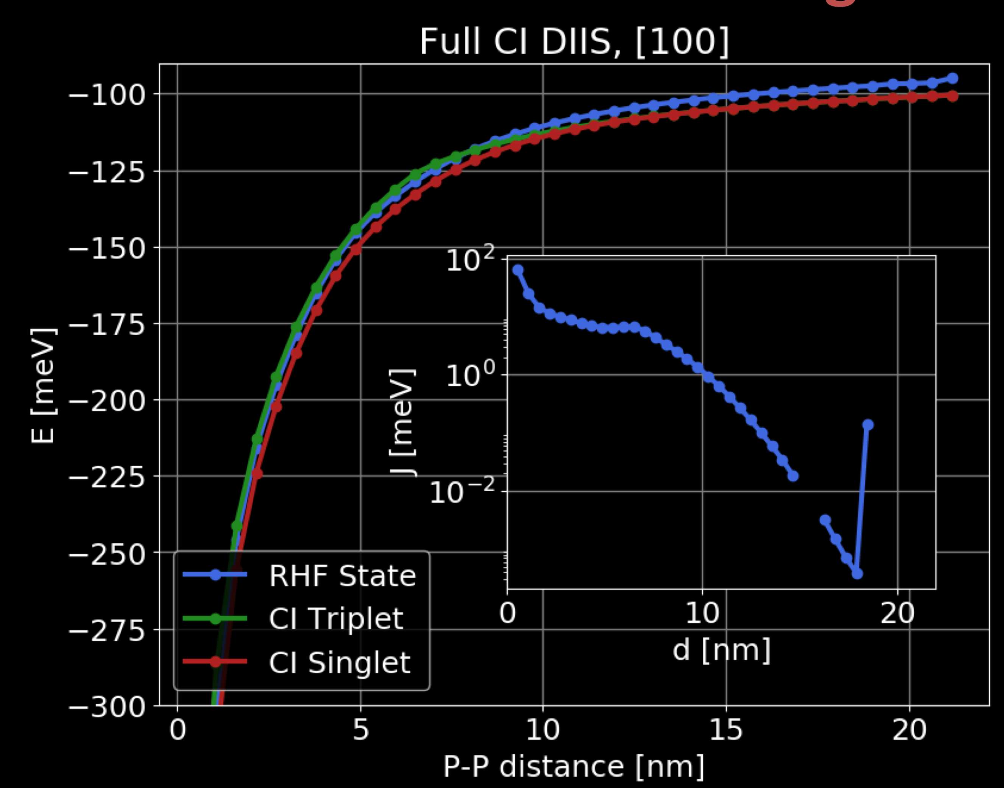
Molecular Orbitals ψ_i ➡ Slater Determinants Φ_j ➡ Many electron WF $\Psi = \sum_i a_i\Phi_i$

RHF ground state: ψ_i … ψ_0 ↑↓ — Φ_0

Excited SDs: ↑ ↓ — Φ_j



4. Exchange Coupled Donors

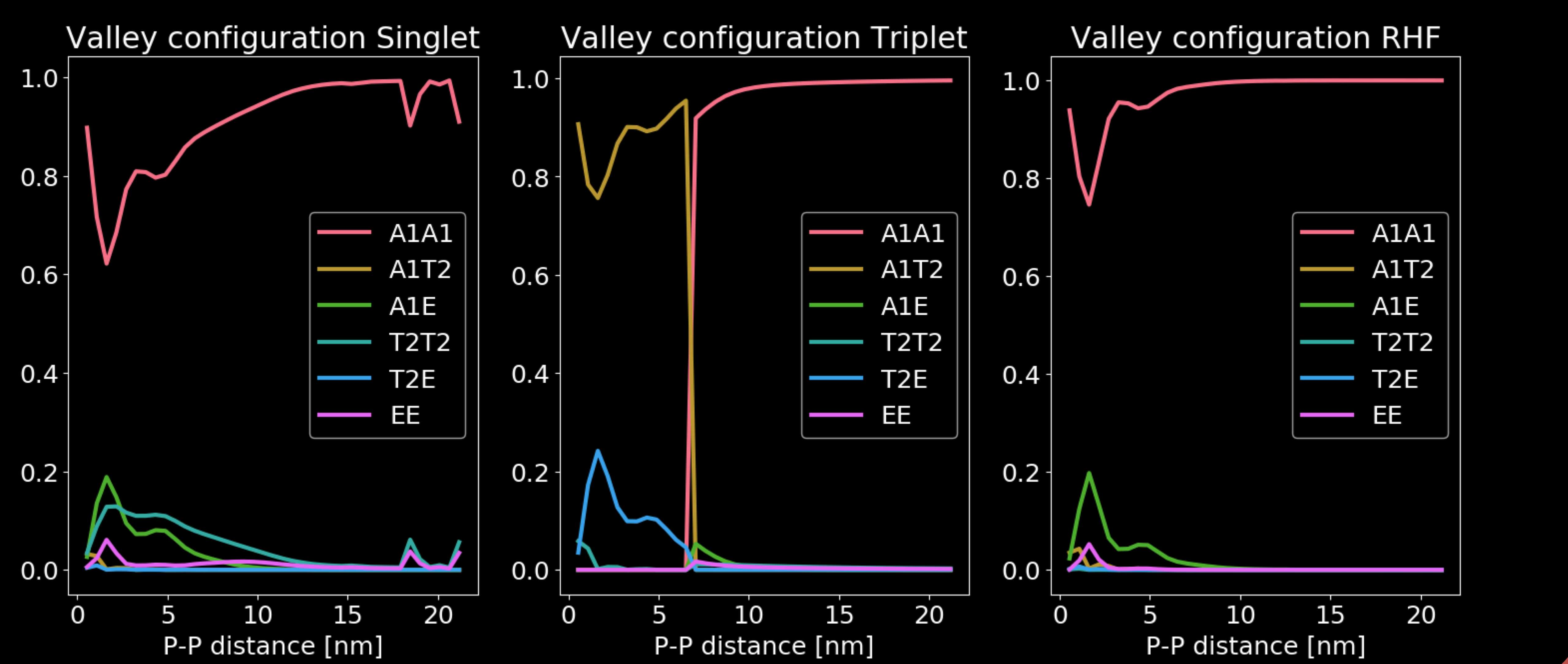


Notable features:

- For large donor distances S and T are A1-like (as expected)
- At 7nm the Triplet mixes in T2
- Below 7nm the exchange appears to evolve non-exponential
- RHF fails for large distances

Future Plans:

- Extend basis to D^--like states
- …



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