

Objective:

- Study Stark Shift of hyperfine coupling
- Compare with experiment, BMB & EMT
- Investigate interface effects for realistic systems
- Establish the physics of quadratic and linear Stark coefficients

Approach:

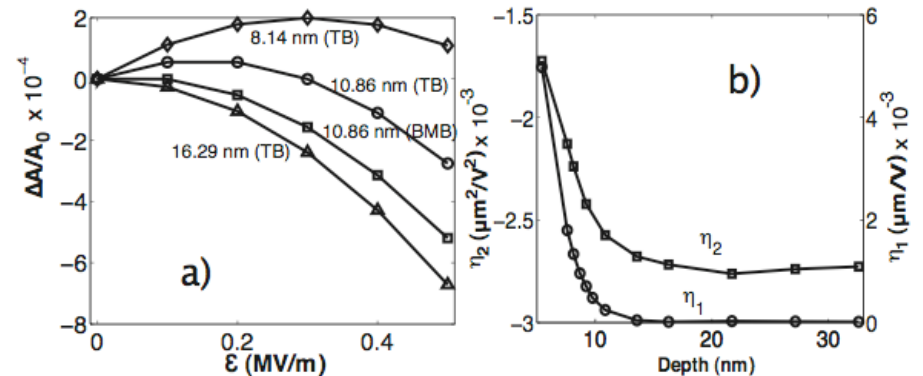
- Use 3.5 M atomistic domain with single P impurity in NEMO 3D under realistic BCs & E-fields
- TB approach optimized for P donors
- Vary impurity depth from interface
- Solve the 20 band spin Hamiltonian by parallel Lanczos algorithm

Results / Impact:

- Quadratic Stark coefficient from TB, BMB & experiment agree well
- EMT estimate differs by an order of magnitude
- Proximity of impurity to interface produces significant linear Stark effect

Left: Field response of hyperfine coupling.

Right: Linear & Quadratic coefficients with Depth



Quadratic Stark Coefficients

Method	Depth (nm)	η_2 ($\mu\text{m}^2/\text{V}^2$)
EXP (Sb)	150	-3.7×10^{-3}
EMT (P)	∞	-2×10^{-2}
BMB (P)	10.86	-2.74×10^{-3}
TB (P)	10.86	-2.57×10^{-3}
	21.72	-2.76×10^{-3}

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