Candidate Muon Stopping Sites in $NaFe_{1-x}Ni_xAs$ and Quantum effects within an anharmonic approximation

Onuorah Ifeanyi John,
Pietro Bonfà, Roberto De Renzi

UNIVERSITÀ DI PARMA

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OUTLINE:

I

- $NaFe_{1-x}Ni_xAs$ (x=0 and 0.5): μSR results, side by side with DFT + local field calculations for muon sites

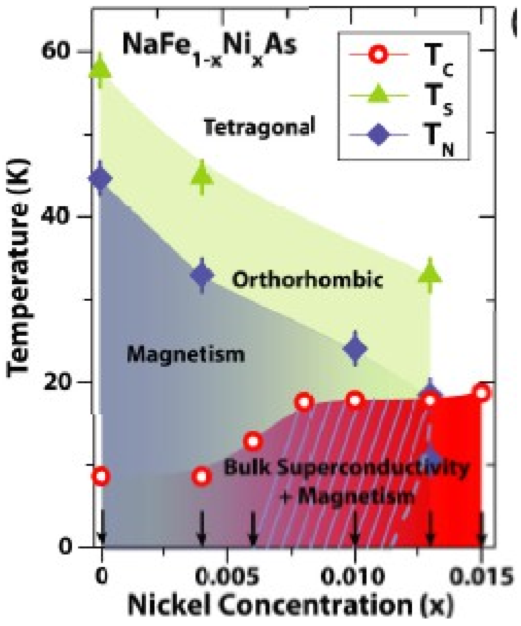
II

- Muon Quantum Effects in B_c of (Fe, Ni, Co) : An approach to include anharmonicity effects in a harmonic muon potential.

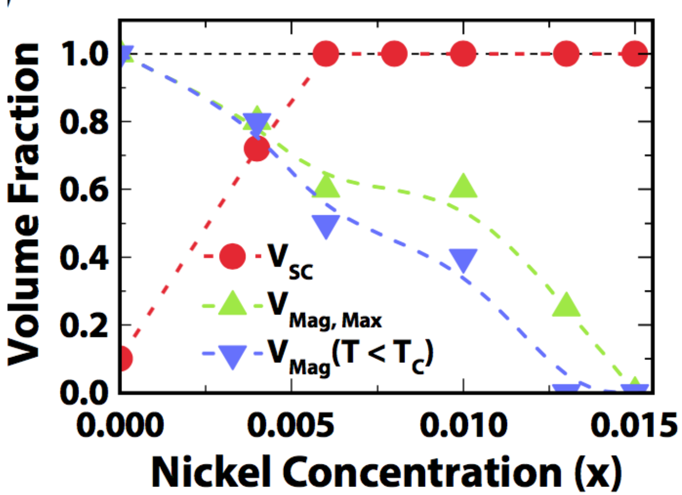
$NaFe_{1-x}Ni_xAs$: Coexistence of magnetism and superconductivity

- Fe-pnictides, with Fe-atoms ordered anti-ferromagnetically
- x= 0% < 0.4%, transition to ~ homogeneous long range magnetically ordered state
- For x=0.4% magnetism is inhomogeneous
- x =1.5% magnetism is completely suppressed

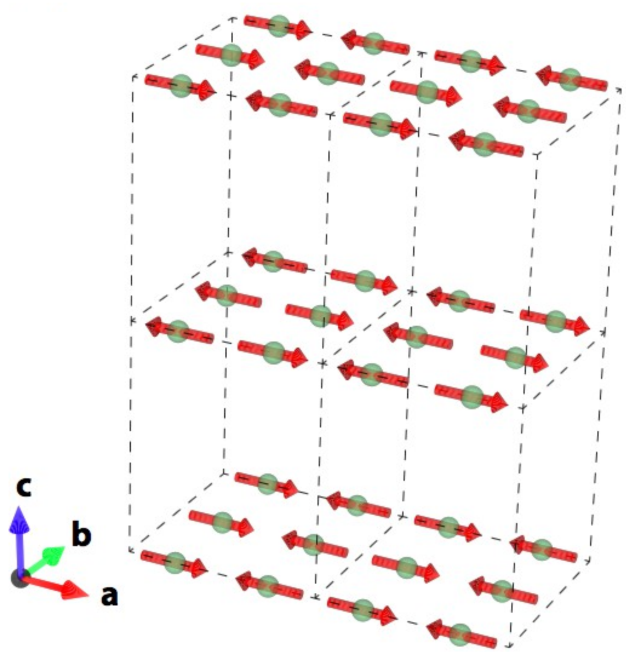
Phase diagram



Magnetic characterization measurements



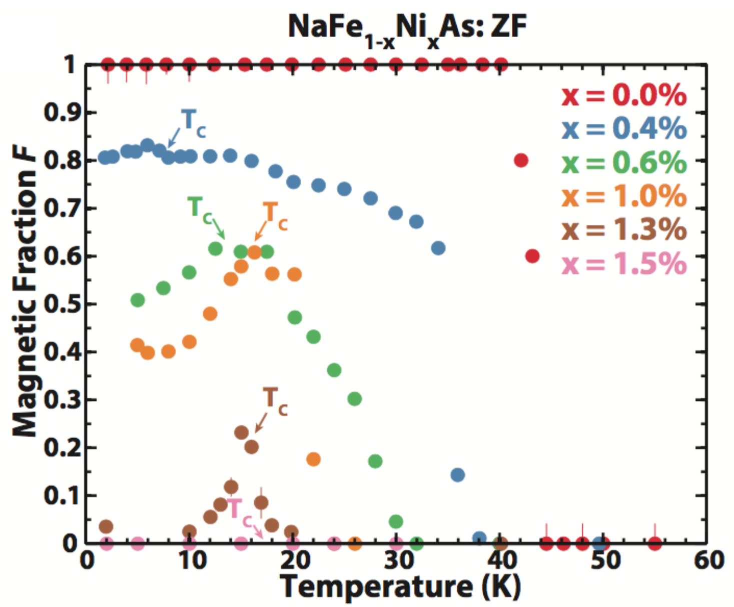
Above measurements by colleagues at Columbia University



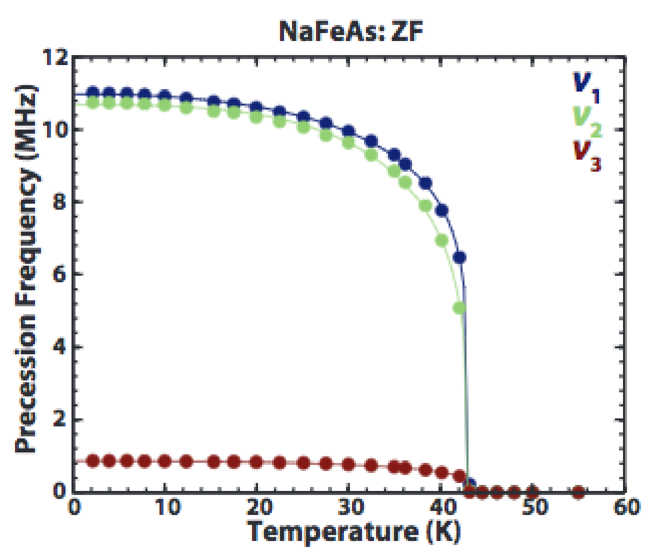
S C. Cheung, et al, PRB 97, 224508 (2018)

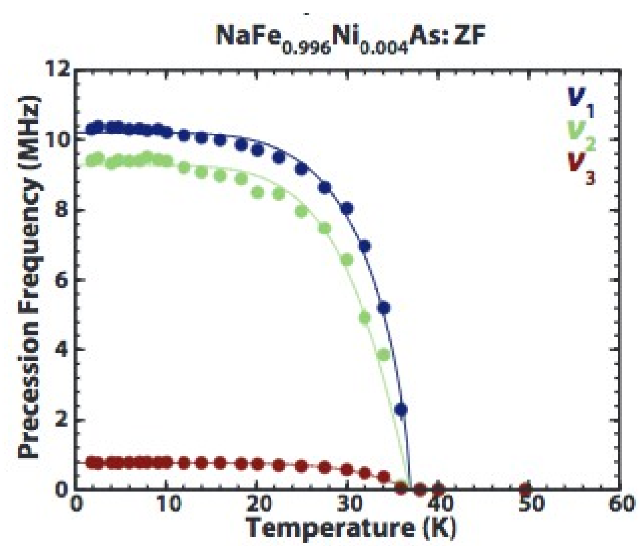
$NaFe_{1-x}Ni_xAs$: ZF-µSR and muon precession frequencies

Evolution of magnetic fraction with T-x



- x =1.5% magnetism is completely suppressed
- Full sample volume is superconducting for x=0.4 %
- Two high precession frequencies and one low frequency

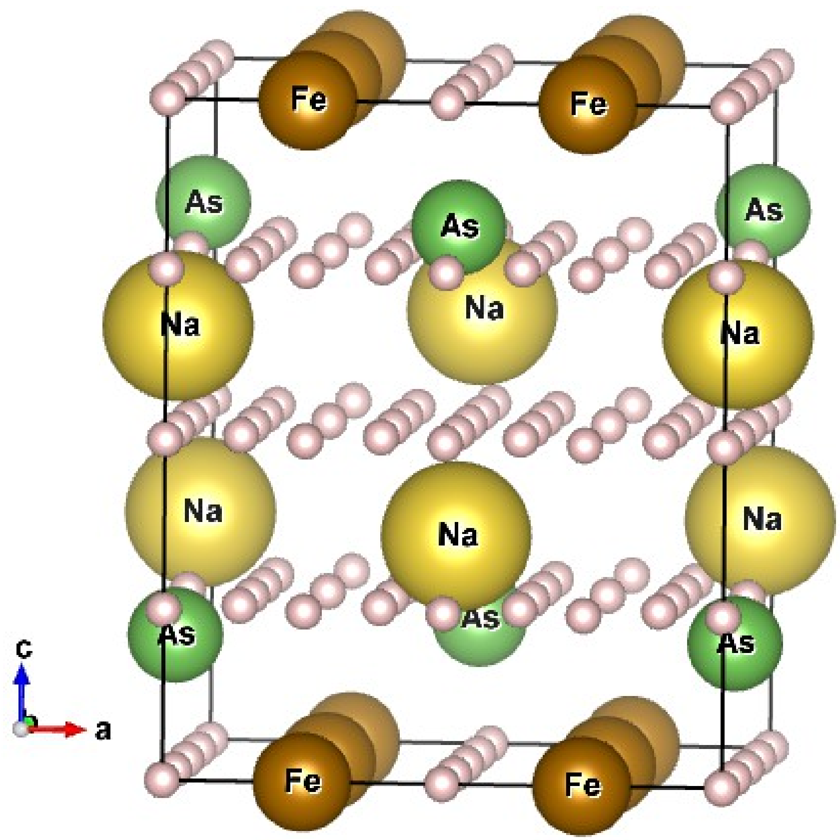




Above measurements by colleagues at Columbia University

$NaFe_{1-x}Ni_xAs$: Starting positions for site search with DFT

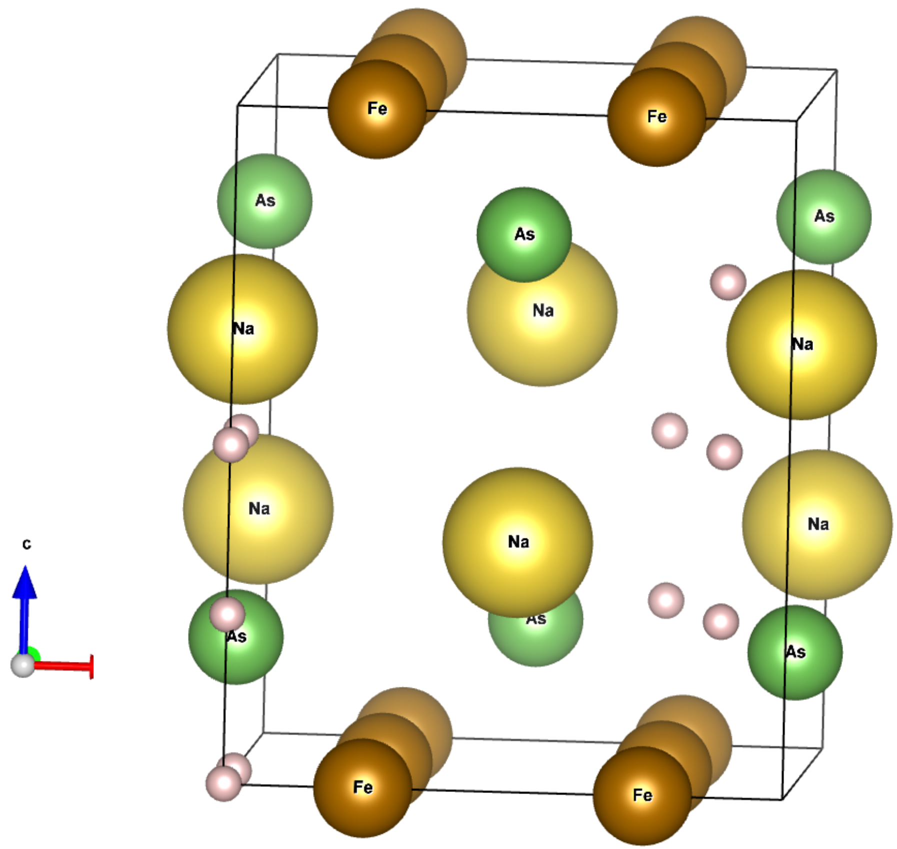
uniform 4 x 4 x 4 muon grid



84 site positions --> 10 symmetrically inequivalent positions.

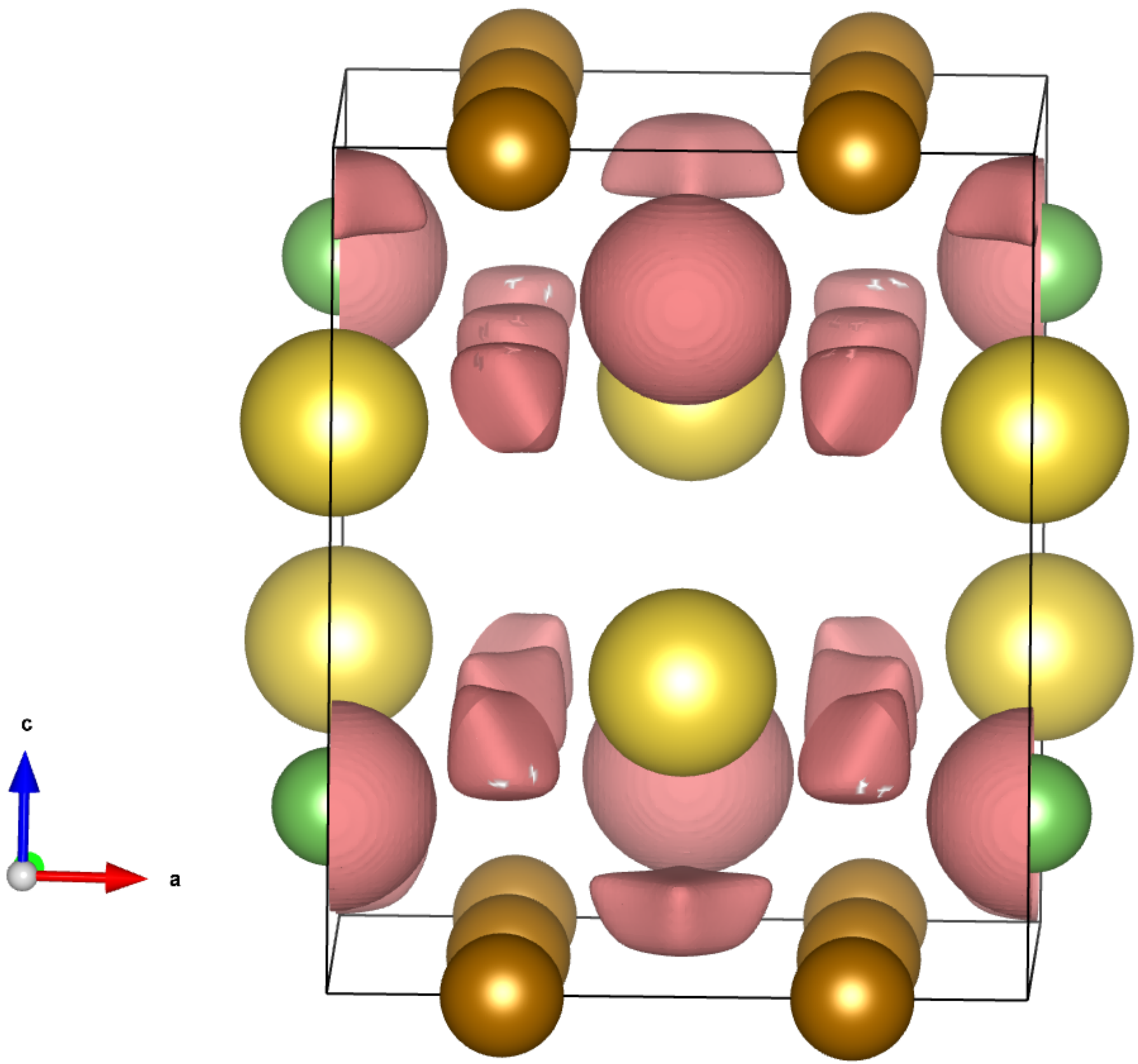
$NaFe_{1-x}Ni_xAs$: Starting positions for search with DFT

10 symmetrically Inequivalent positions.



NaFe$_{1-x}$Ni$_x$As: Starting positions for site search with DFT

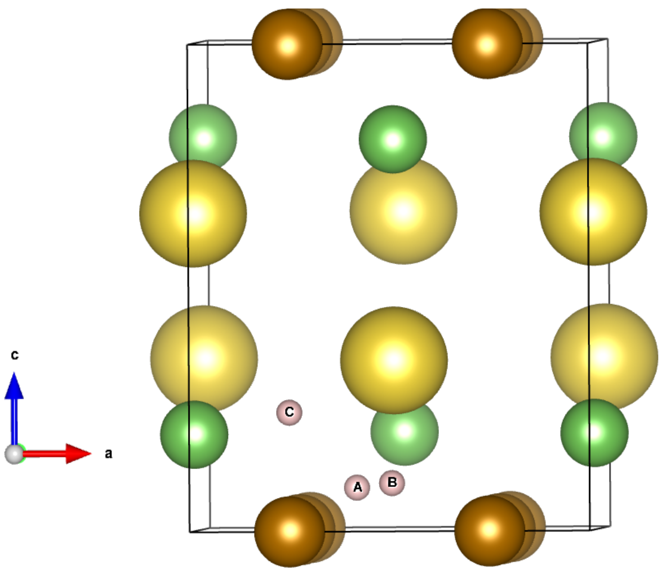
+ 2 positions of unperturbed electrostatic potential minima



$NaFe_{1-x}Ni_xAs$: Candidate muon sites

- Total energy and Forces between atoms are converged to a threshold of 1e-4 with DFT within the 2x2x2 supercell

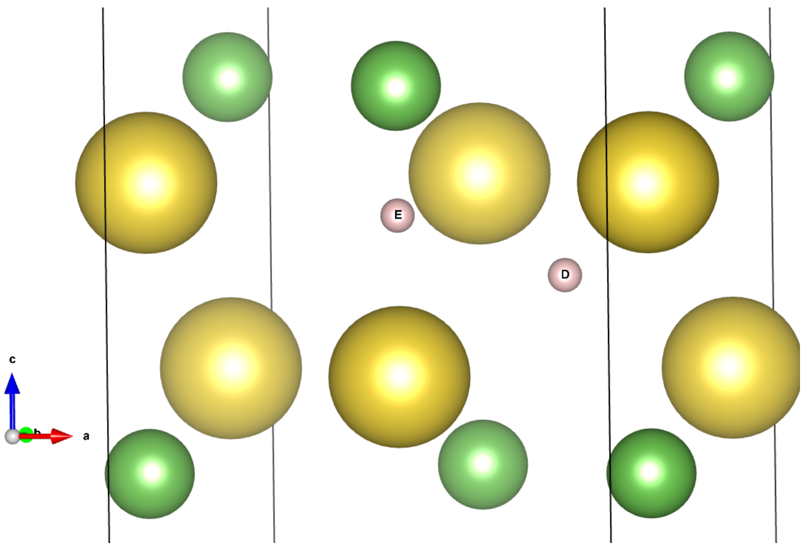
	Label	Symm	Site Positions	ΔE (meV)
Cluster I	A	8n	(0.41, 0.25, 0 .10)	0
	B	8m	(0.50, 0.12, 0.10)	42
	C	8l	(0.25, 0.01, 0.25)	183
Cluster II	D	4b	(0.75, 0.50, 0.50)	287
	E	4g	(0.50, 0.25, 0.60)	436

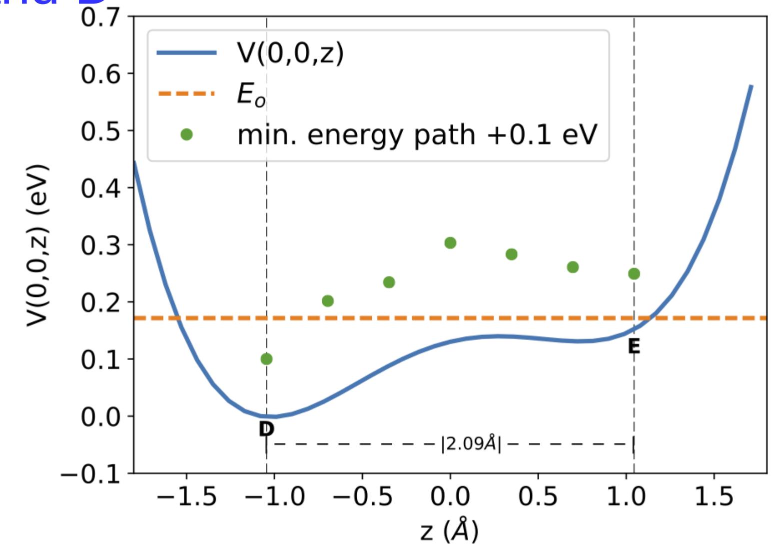


- Clusters grouped considering DFT energy and simulated frequencies
- Calculations for $NaFe_{0.5}Ni_{0.5}AS$ results in similar candidate muon sites

$NaFe_{1-x}Ni_xAs$: Candidate sites: Cluster II

NEB + model barrier for Sites E and D





Plot V(0,0,z) Toy model potential

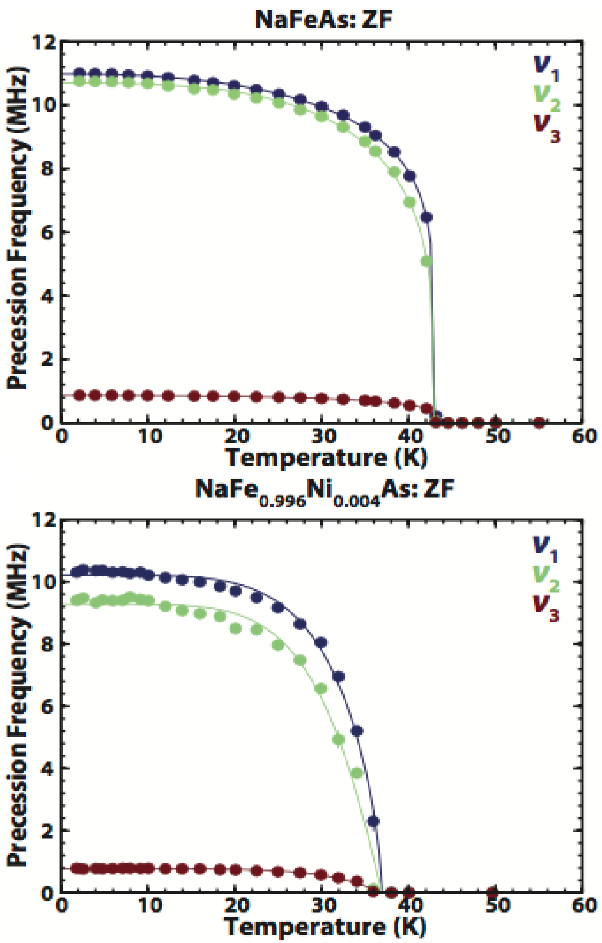
- $V(x,y,z)= 1/2a(x^2+y^2)+1/2(bz^4 - c\,z^2 + dz) + f$

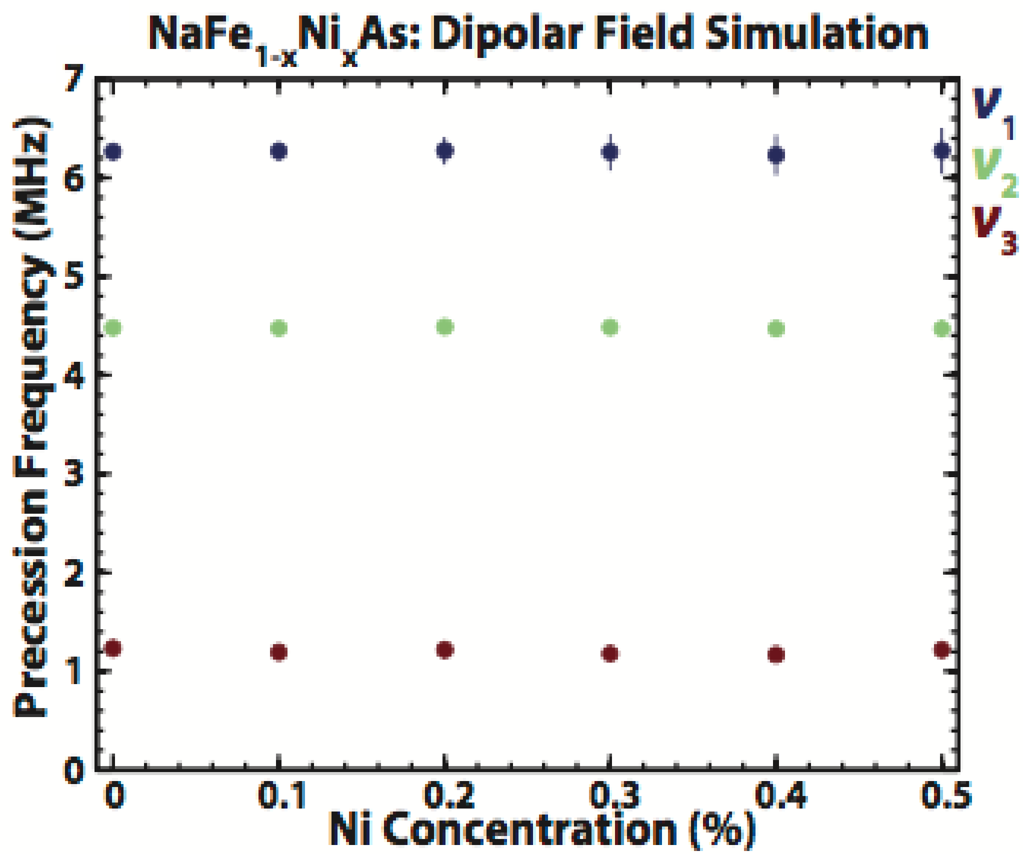
With constants, $a=2.44 \times 10^{-3}$ $b=5.04 \times 10^{-4}$, $c= 3 \times 10^{-3}$, $d=2.85 \times 10^{-3}$, $f= 4.79 \times 10^{-3}$ all in Hartree units.

- Suggests delocalization of the muon over sites D and E.
- 3 sites--> B, A and < D and E>. For C highly unstable.

$NaFe_{1-x}Ni_xAs$: Local fields at the muon

Dipolar sum at the muon: $$B_{dipole}(r_\mu) = \sum_i \left(\frac{\mu(r_i)}{(|r_i - r_\mu|)^3} - \frac{3(r_i - r_\mu)(\mu(r_i).(r_i - r_\mu))}{(|r_i - r_\mu|)^5} \right)$$





- Estimated Fe magnetic moment with site B, approx. 0.175 μ_B. Comparable to 0.17 μ_B of neutron scattering and 0.15 μ_B of Mössbauer.

Quantum Effects of the muon: Contact hyperfine field

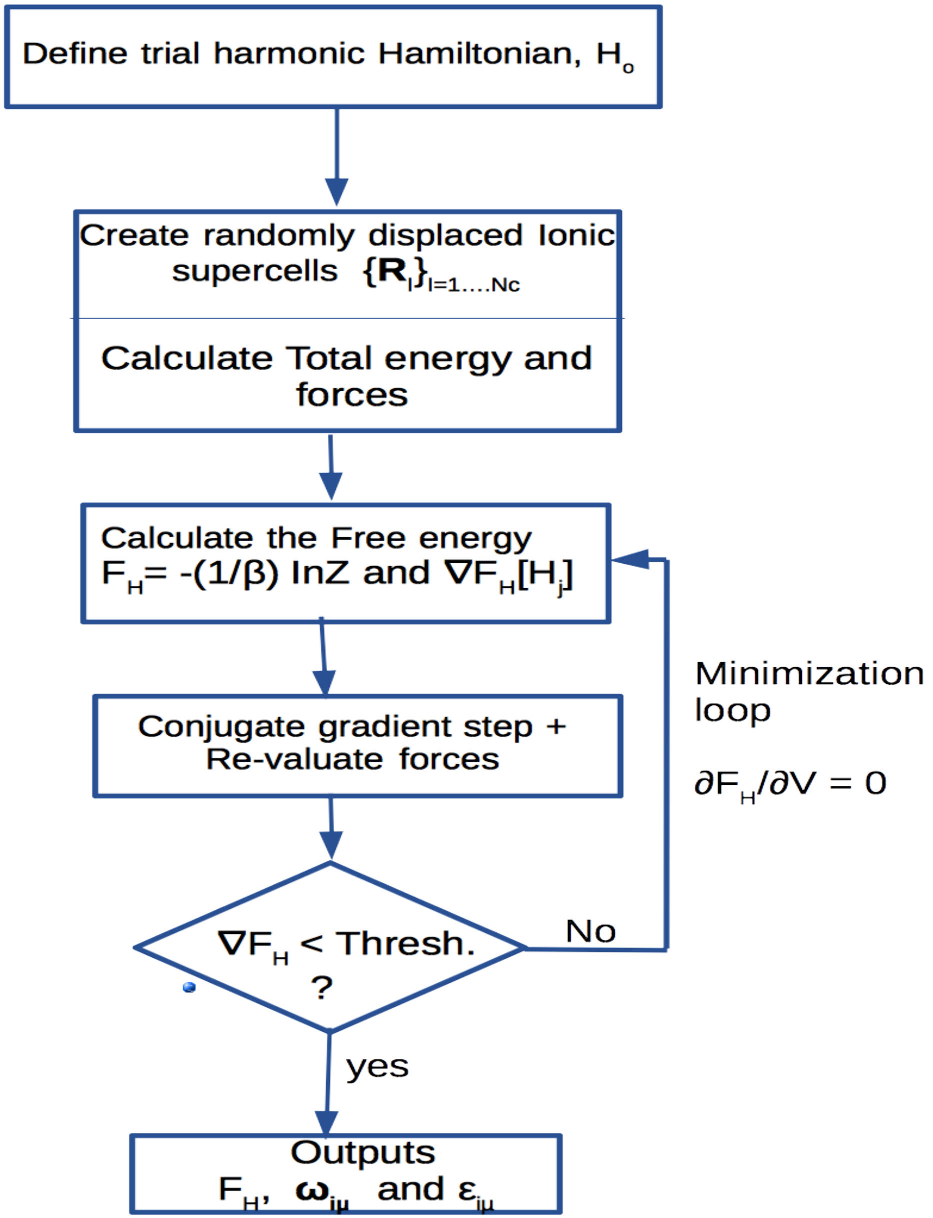
- DFT within Born-Oppenheimer approx. does not treat electrons and the nuclei on same footing. Light mass of the muon not considered.

- To a first approximation the muon potential is treated with a harmonic potential, but the muon potential is not harmonic.

- Include anharmonicity in the description of the muon potential

Quantum Effects of the muon: Anharmonicity within a self - consistent Harmonic approximation (SCHA)

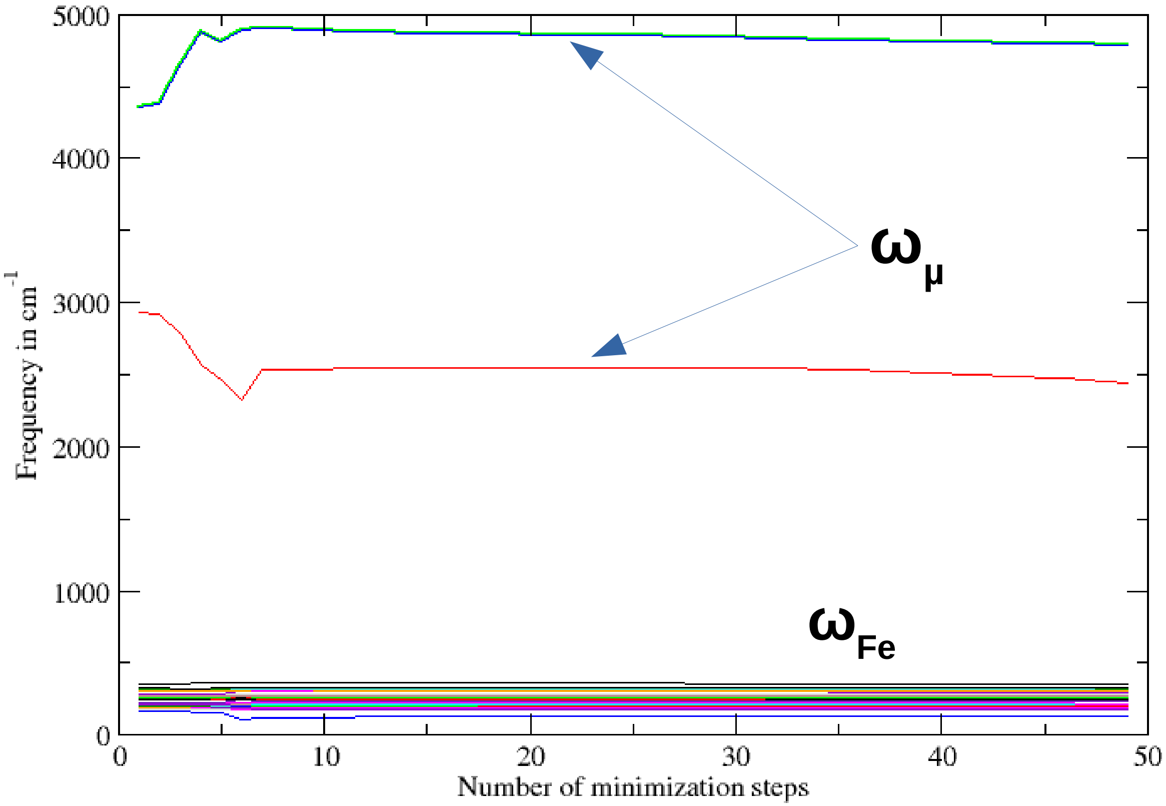
Summary of the approach:

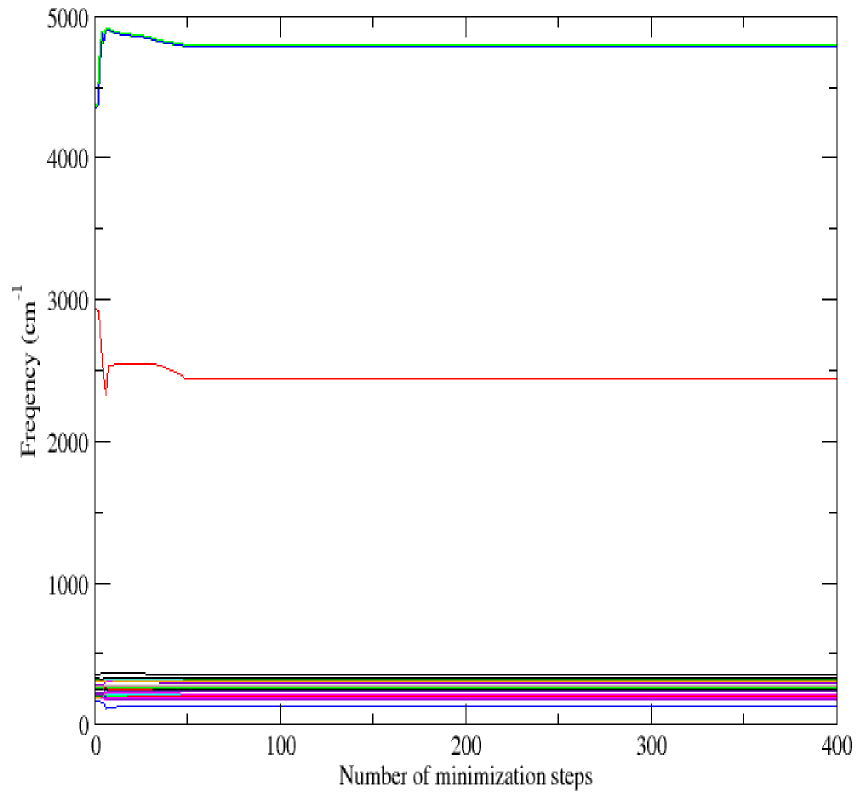


I. Errea etal, PRL 111, 177002 (2013)

Quantum Effects of the muon: 'Effective' harmonic approximation

Frequency evolution during free energy minimization (μ - Fe-bcc)





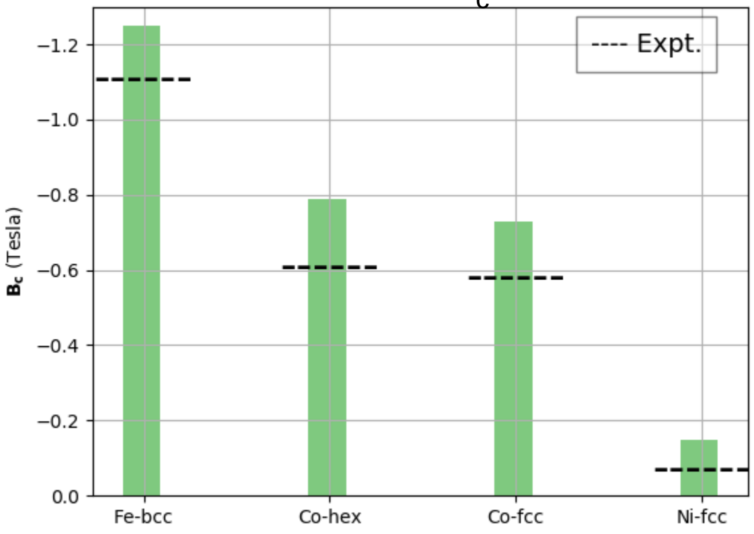
- Because of difficulty in parameterizing the anharmonicity, till now we still have a harmonic potential but with an effective frequency, $\omega_{effective}$

Quantum Effects of the muon: Contact hyperfine field

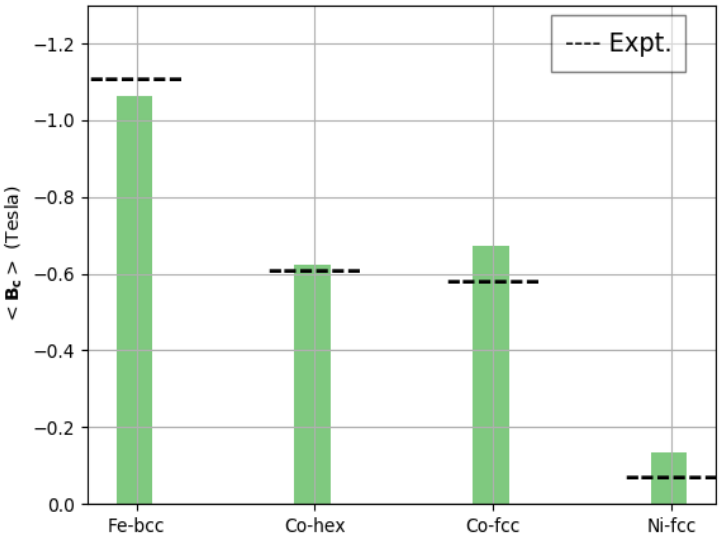
	E_o (eV)	
	Harmonic	Anharmonic
Fe(bcc)	0.72	0.77
Co(hcp)	0.53	0.68
Co(fcc)	0.49	0.64
Ni(fcc)	0.44	0.62

$$\langle B_c \rangle = \int |\psi(\mathbf{r})|^2 B_c(\mathbf{r}) dr$$

Static B_c



Averaged B_c



I. J. Onuorah et al, PRB 97, 174414 (2018)

Thanks