Density-Functional Theory Calculations Relevant to Hydride Formation and Prevention

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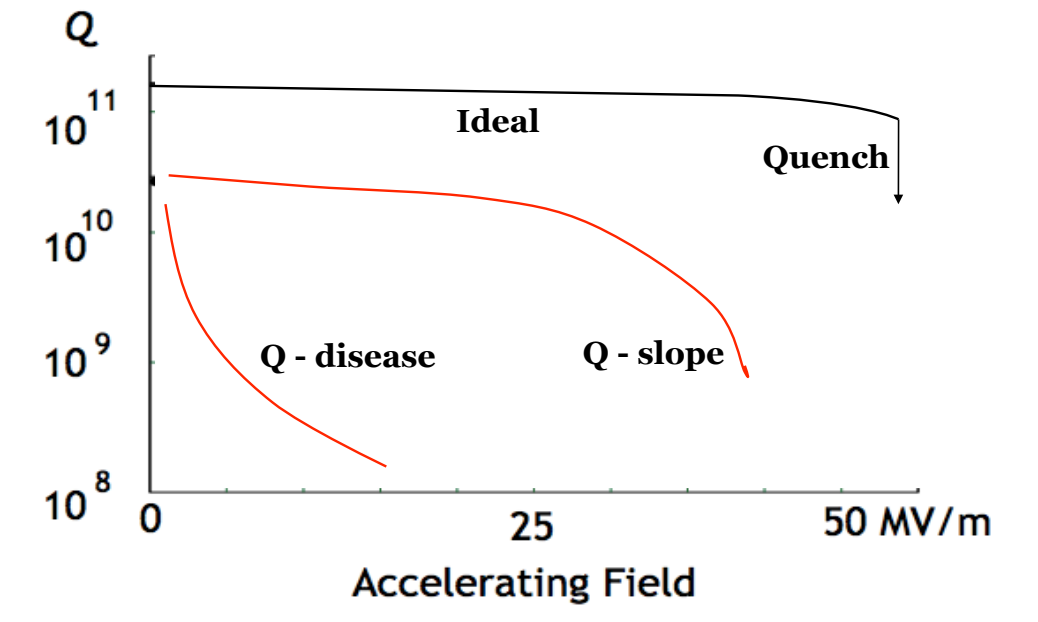
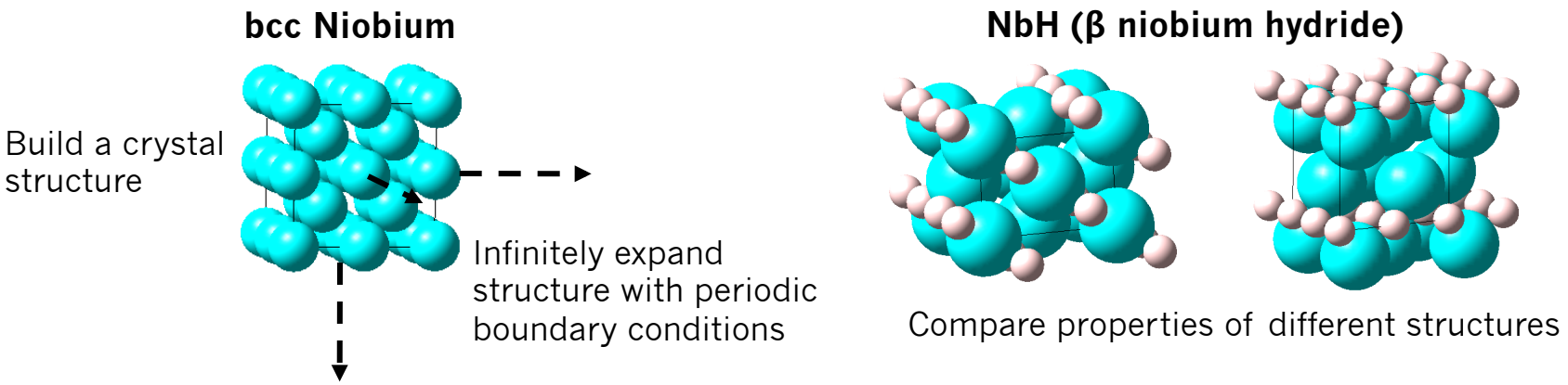
SRF Cavity Limitations Related to Impurities in Niobium



Impurities can

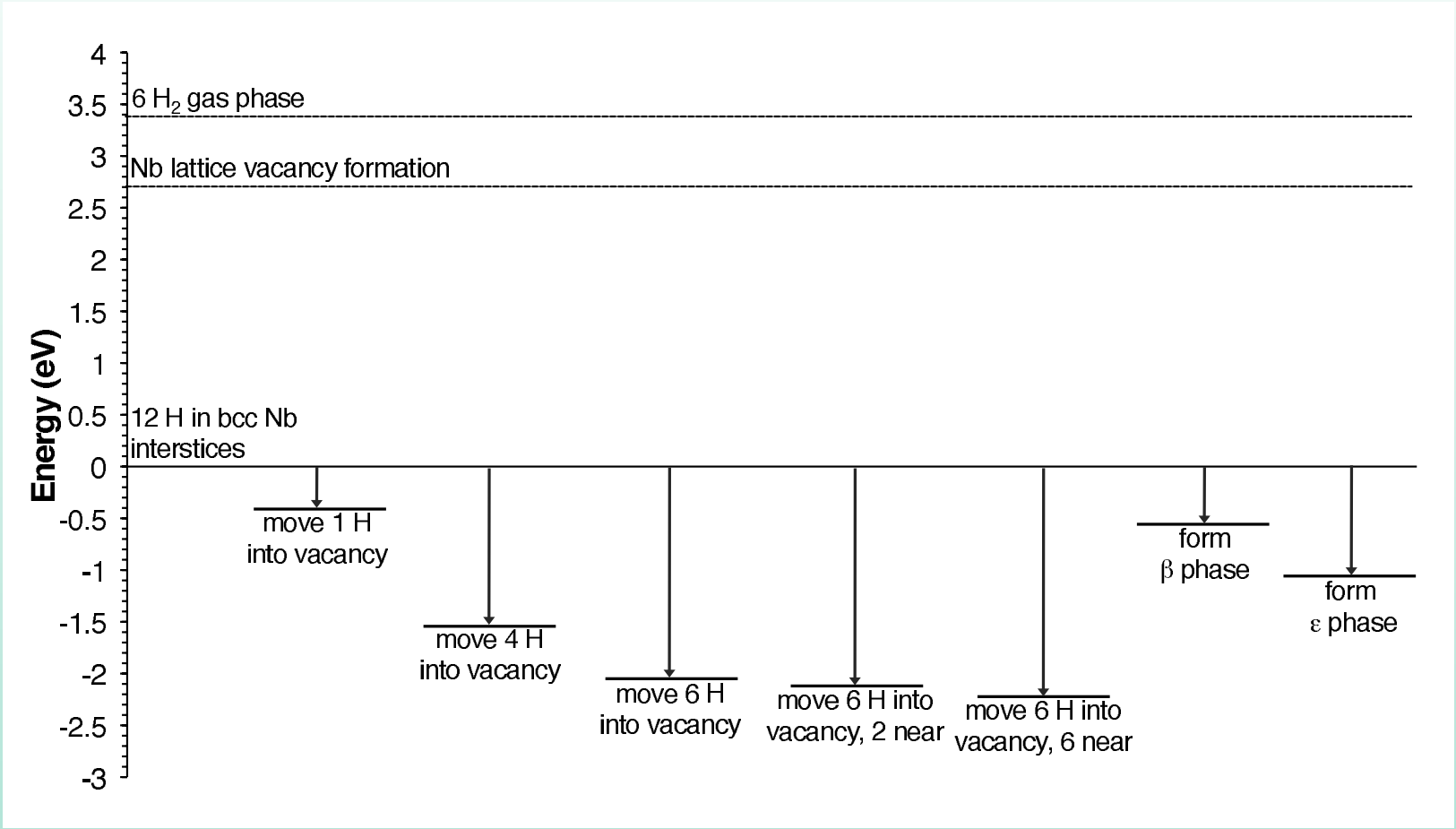
- be dissolved in the metal and cause reduction of T_c and local heating
- form precipitates with local magnetic moments or reduced T_c

Density Functional Theory Modeling



- Solve the electronic structure problem for the model systems using DFT in VASP
- Assess properties such as binding energy, charge distribution, and niobium lattice strain

Hydride Phase Formation



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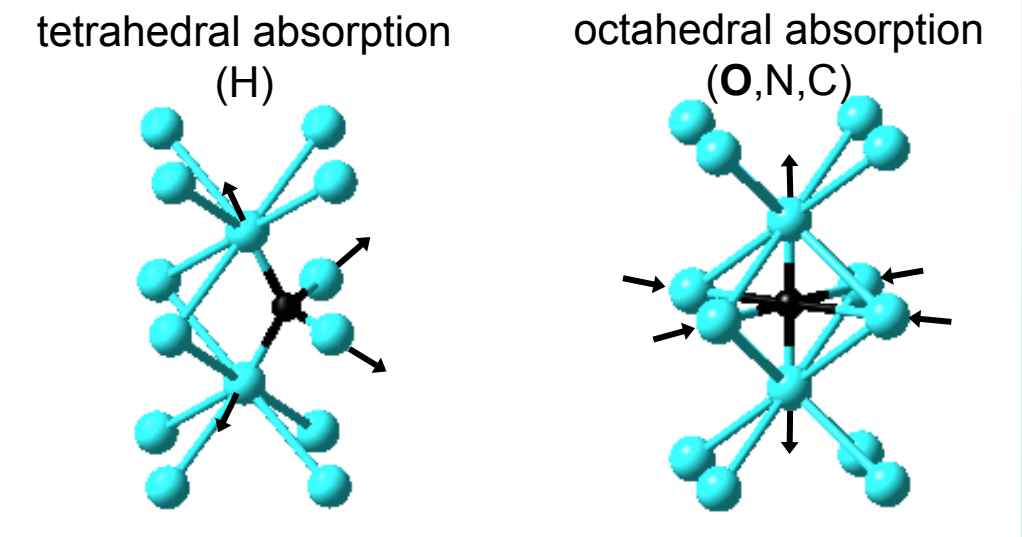
Interstitial Hydrogen, Oxygen, Nitrogen, and Carbon



	$Nb_{128}H$	$Nb_{128}O$	$Nb_{128}N$	$Nb_{128}C$
Charge on interstitial atom (e^-)	-0.65	-1.35	-1.63	-1.76
Binding energy (eV)	-2.41	-7.02	-7.39	-8.48
Lattice strain energy (eV)	0.11	0.83	0.83	0.96

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Hydride Phase Prevention by Absorbed Oxygen

- Further examination of oxygen showed
  - Interstitial oxygen traps interstitial hydrogen
  - Oxygen preferentially migrates to niobium site vacancies over hydrogen
- Mechanism for the low temperature bake (which mitigates Q-slope)
  - -> Break up hydride phases
  - -> Detrap hydrogen from niobium lattice defects
  - -> Block phase nucleation sites with oxygen atoms
  - -> Trap interstitial hydrogen with interstitial oxygen atoms
- Would nitrogen have a similar effect?

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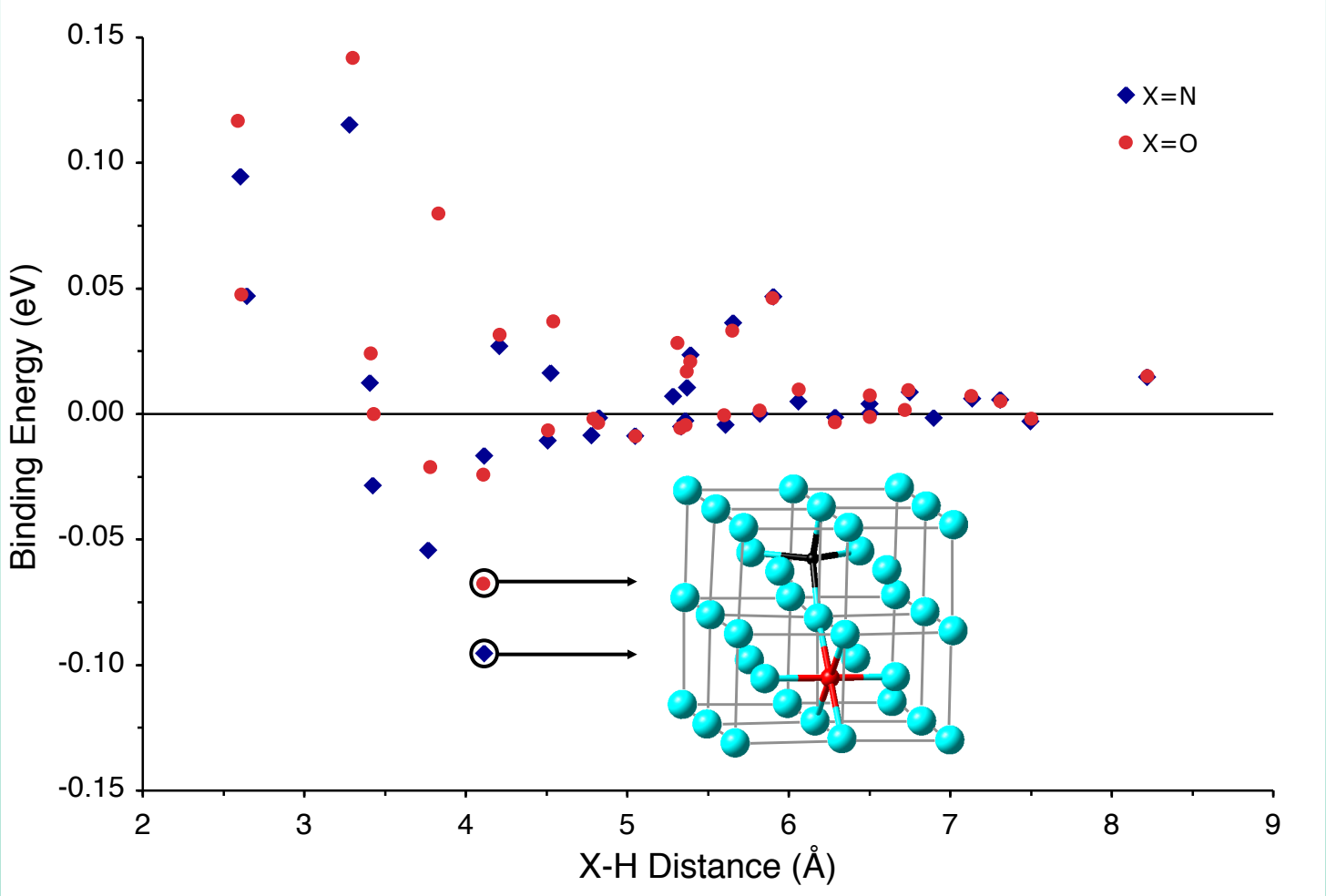
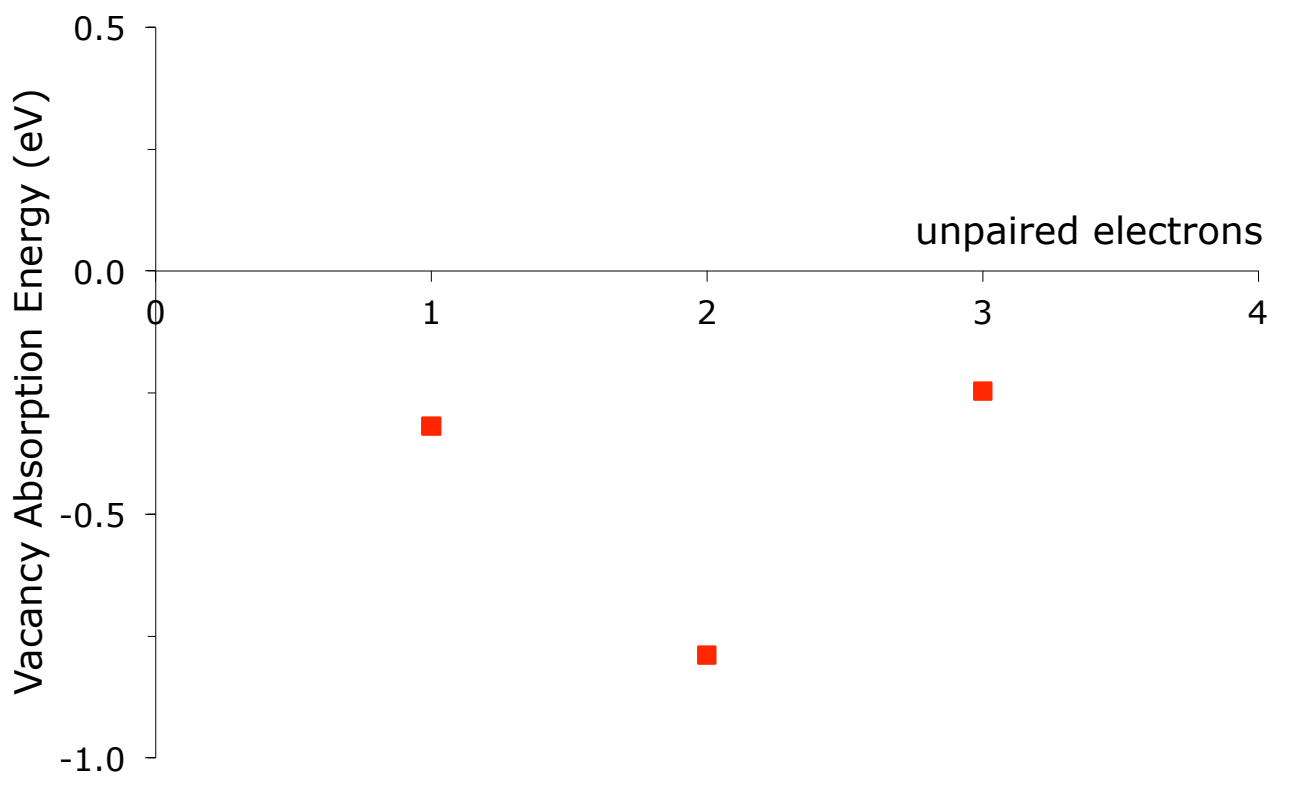
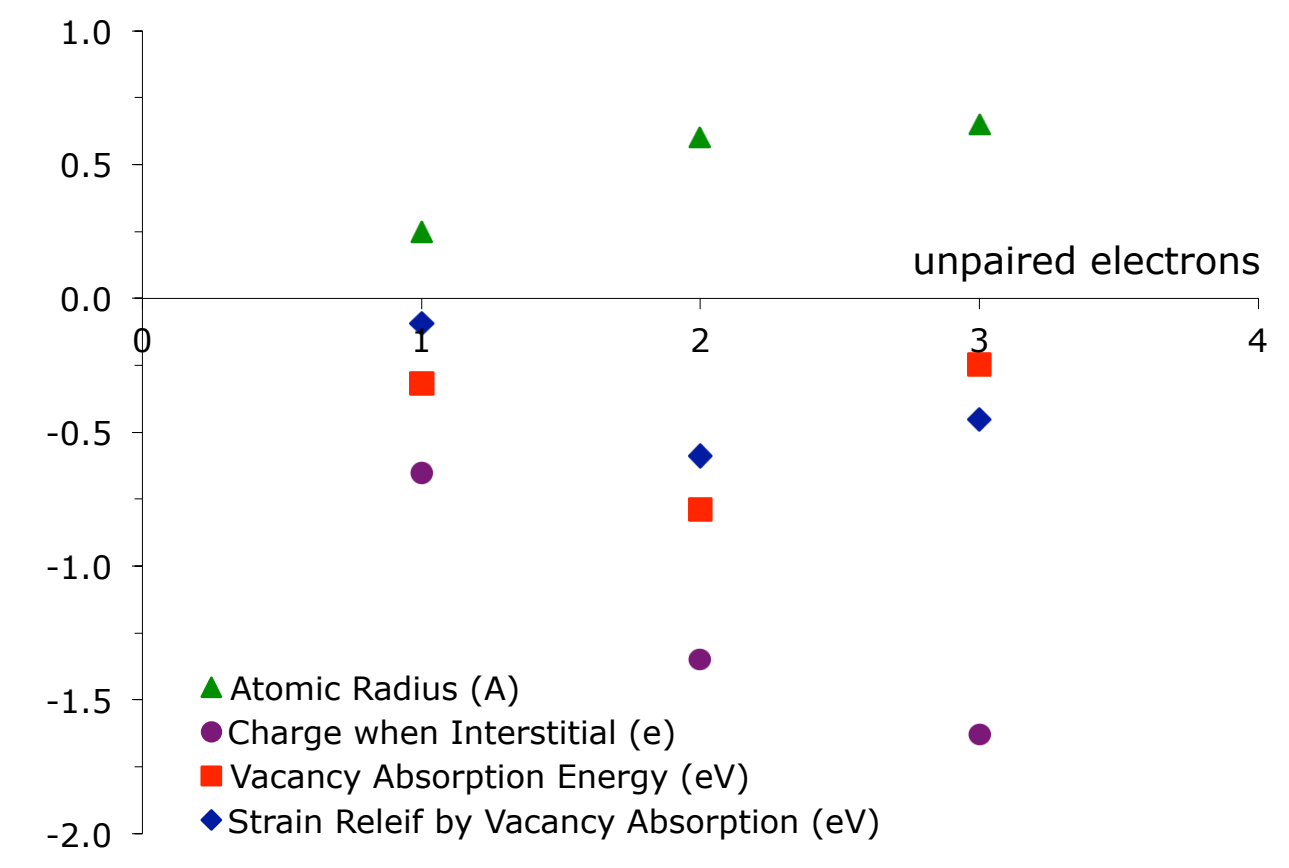
Hydrogen Trapping by Oxygen and Nitrogen



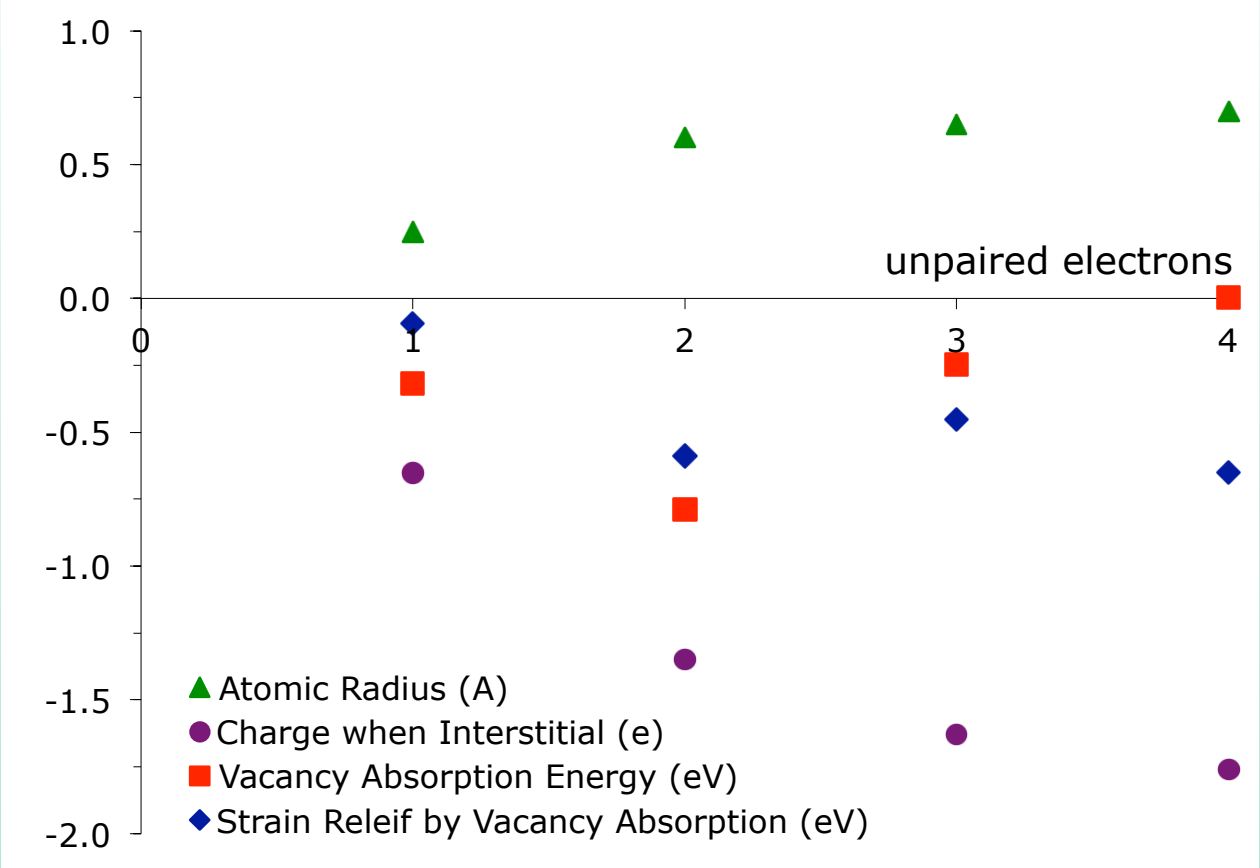
Hydrogen, Oxygen, and Nitrogen in Niobium Site Vacancies



Hydrogen, Oxygen, and Nitrogen in Niobium Site Vacancies



Hydrogen, Oxygen, Nitrogen, and Carbon in Niobium Site Vacancies



Hydrogen, Oxygen, and Nitrogen in Niobium

- Vacancy trapping and detrapping energies[1,2,3] :

  N>O>H

- Effect on superconducting transition temperature[4,5,6]
  - O>N>H
  - hydride precipitates $T_c < 2$ K
  - some nitrides $T_c > 10$ K

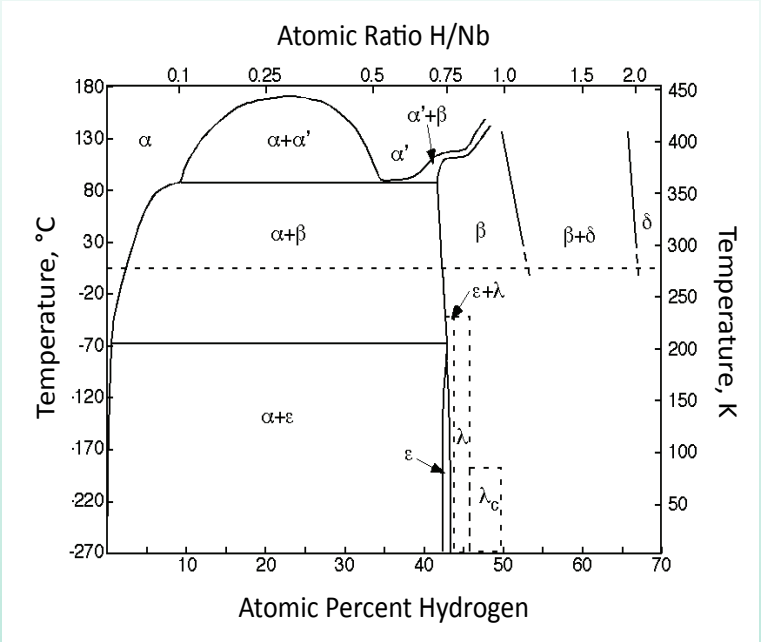
1. Hautojarvi P, et al. 1985 Phys. Rev. B 32 4326–31; 2. Igata N, Miyahara K, Ohno K and Hakomori K 1982 J. Nucl. Mater. 108/109 234–9; 3. Wechsler M S and Murty K L 1989 Metall. Trans. A 20A 2637–49; 4. DeSorbo W 1963 Phys. Rev. 132 107–23; 5. Jisrawi N M, et al. 1998 Phys. Rev. B 58 6585–90; 6. Ohlendorf D and Wicke E 1979 J. Phys. Chem. Solids 40 721–8

Conclusions

- Suggested improvements for processing
  - Tailor bake temperature and time to eliminate hydride precipitates and supply the appropriate amount of oxygen to prevent their reformation
  - Potentially use nitrogen for milder effect on superconducting transition temperature
- Future work
  - Examine the formation of nitride phases in niobium
  - Examine the effect of various Nb_xN_y, $Nb_xN_yH_z$, $Nb_xO_yH_z$ complexes on the superconducting properties of the niobium
  - Examine the role of dislocations in hydride phase formation/prevention

Hydrogen in Niobium

- α, α’ – interstitial hydrogen dispersed in bcc niobium
- β, ε – ordered hydrogen interstitials in fco niobium
- δ – ordered hydrogen interstitials in fcc niobium – fluorite structure
- λ, λ_c – experimentally unconfirmed phases



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Density Functional Theory Modeling

- Solve the electronic structure problem for the model system
- Parameters
  - Vienna Ab Initio Simulation Package (VASP)
  - Plane wave basis set w/400 eV cutoff
  - PAW pseudopotentials to describe atomic cores
  - PBE-GGA exchange-correlation functional
  - 0.25/Å gamma-centered *k*-point mesh
- Bader Method to assign local properties