

High-Throughput and Ab Initio Molecular Dynamics approaches for Developing Alloy Diffusion Databases (with an Application to Radiation Induced Segregation in Ni-Cr Alloys)

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Multicomponent Diffusion Data and Its Impact on the Materials Design Process: Data Needed; Data Acquisition; and Data Application

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Outline

- Some thoughts on Ab-Initio Diffusion Calculations
- Simple Diffusion in Elements/Dilute alloys
 - High-throughput approaches
- Screening for Fast Oxygen Migration in Perovskites
 - High-throughput and datamining
- Ni-Cr Radiation Induced Segregation
 - Ab initio MD approach
- Summary

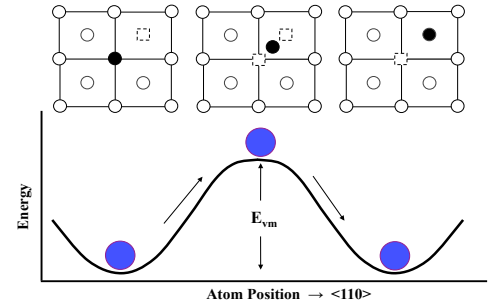
Some Thoughts on Opportunities in Ab-Initio Diffusion Calculations

- Simple diffusion (no or limited structural/chemical disorder)
 - Pure elements, pure sublattices in ordered phases, dilute impurities, simple surfaces, ...
 - Ab initio (CNEB + Phonons) + Analytic models => D
 - Opportunities for high-throughput/datamining approaches
- Complex diffusion (structural/chemical disorder)
 - Concentrated alloys, grain boundaries, interfaces, clusters, ...
 - Ab initio (CNEB + Phonons) + Kinetic Monte Carlo => D
 - Molecular Dynamics (for “low” barriers ~ 0.5 eV) => D

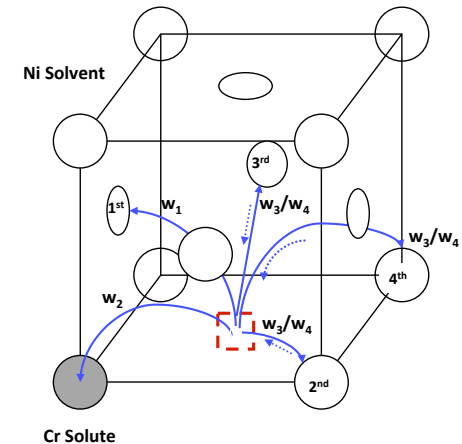
Simple Diffusion in Elements/Dilute Alloys: High-Throughput Approaches

Basic Vacancy Diffusion for Pure Elements, Dilute Alloys

- **Diffusion in pure elements:**
 - Dominated by a single defect formation and migration energy taking ~ 10 hours to predict
- **Diffusion in dilute alloys:** multi-frequency models can predict D accurately
 - Dominated by ~ 5 defect and migration energies taking few days to predict



$$D = a^2 f \nu \exp\left(-\left(E_{vf} + E_m\right)/kT\right)$$



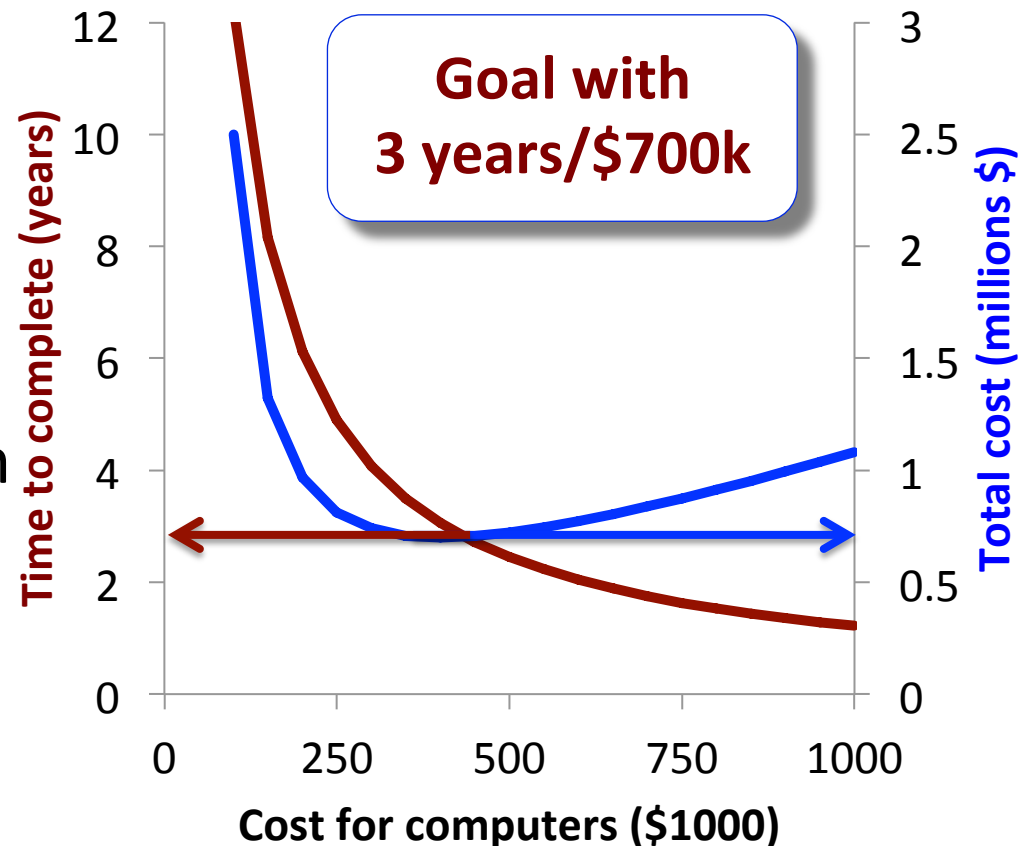
Opportunity for database development with high-throughput calculations

High-Throughput for Pure Elements, Dilute Alloys – A Materials Genome Opportunity

Determine D^* for pure A and $A_{1-x}B_x$ ($x \ll 1$) for all elements in the FCC, BCC, and HCP crystal structures

Resource needs

- ~40 viable pure elemental systems in each structure → 2,500 alloy-structure systems
- 1 system takes ~5 day on 100 cores (= \$20k).
- So need about 3,500 Core-Years, 1 postdoc.



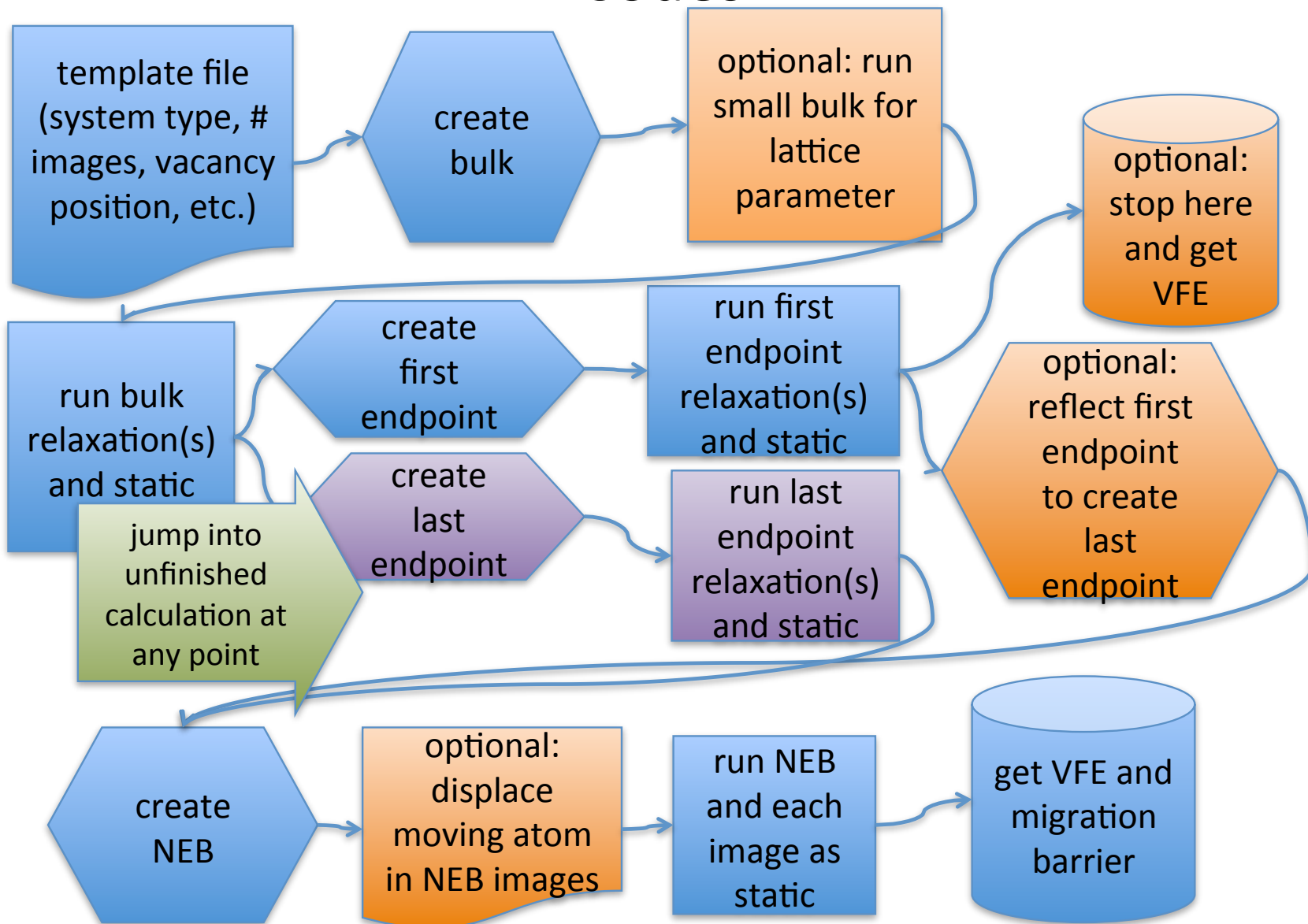
Present Efforts: High-Throughput for Pure Elements

Evaluate diffusion activation energy for all pure elements in all three crystal structures (HCP, BCC, FCC)

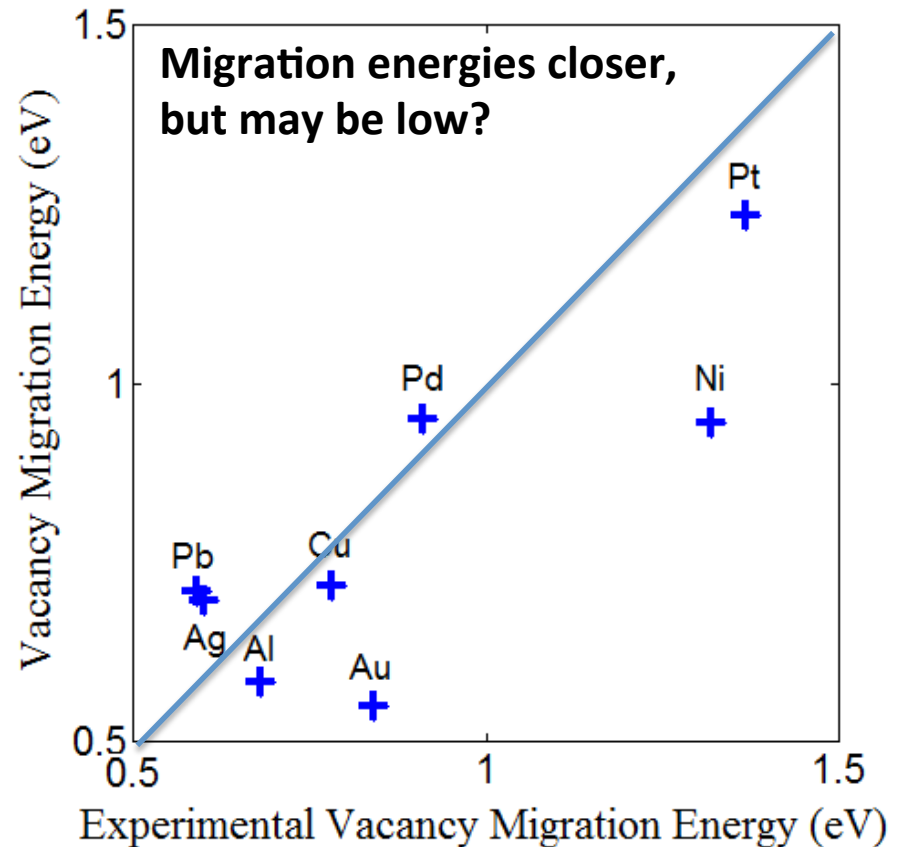
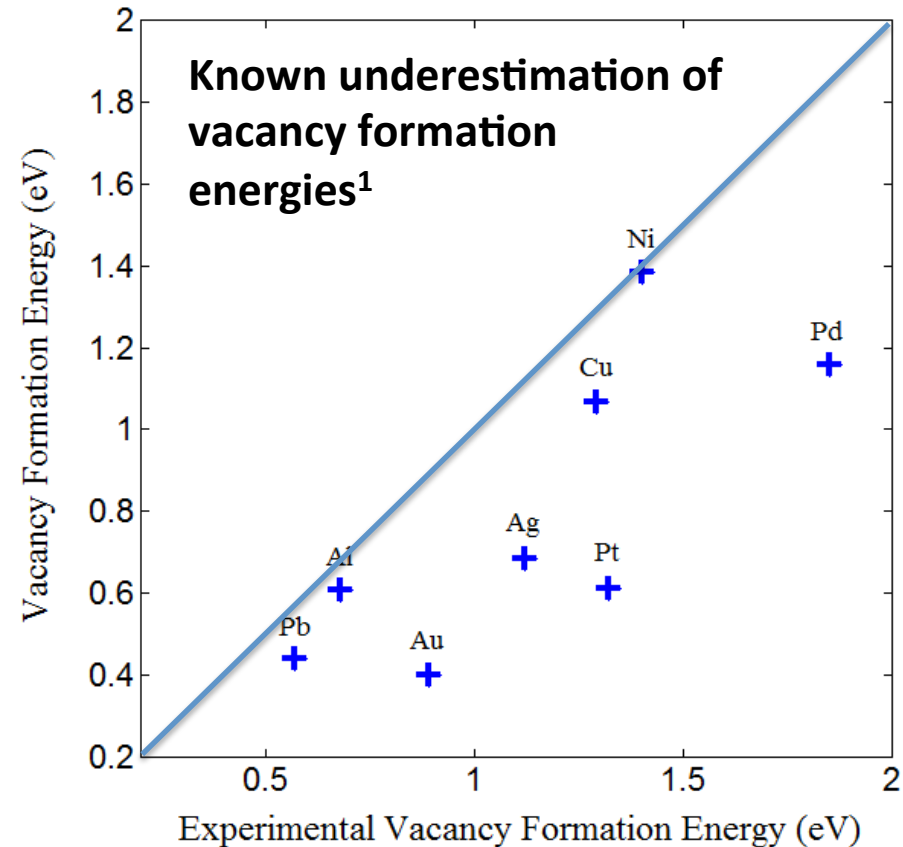
Status

- Written automation codes to perform high-throughput computations
- # Completed Evac calculations = 47 hcp + 48 fcc = 95
- # Completed Emig calculations = 24 hcp + 43 fcc = 67
- Rate of Completion has been ~ 1 system/day on 100 cores
- All calculations with DFT from VASP, GGA, PAW
- **Work done with one undergraduate guided by a graduate student**

High-Throughput Diffusion Calculations – Python Codes

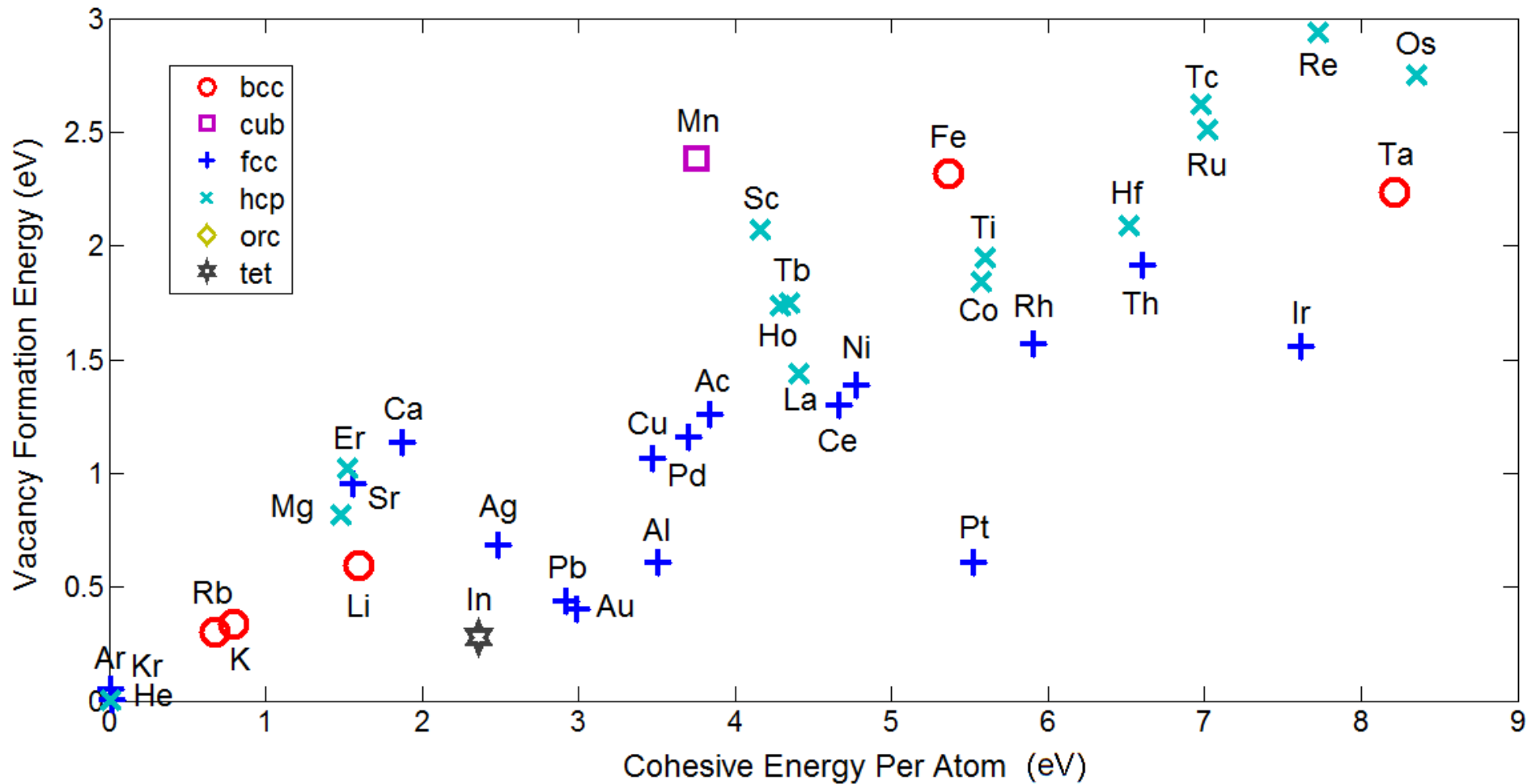


Trends vs. Experiment

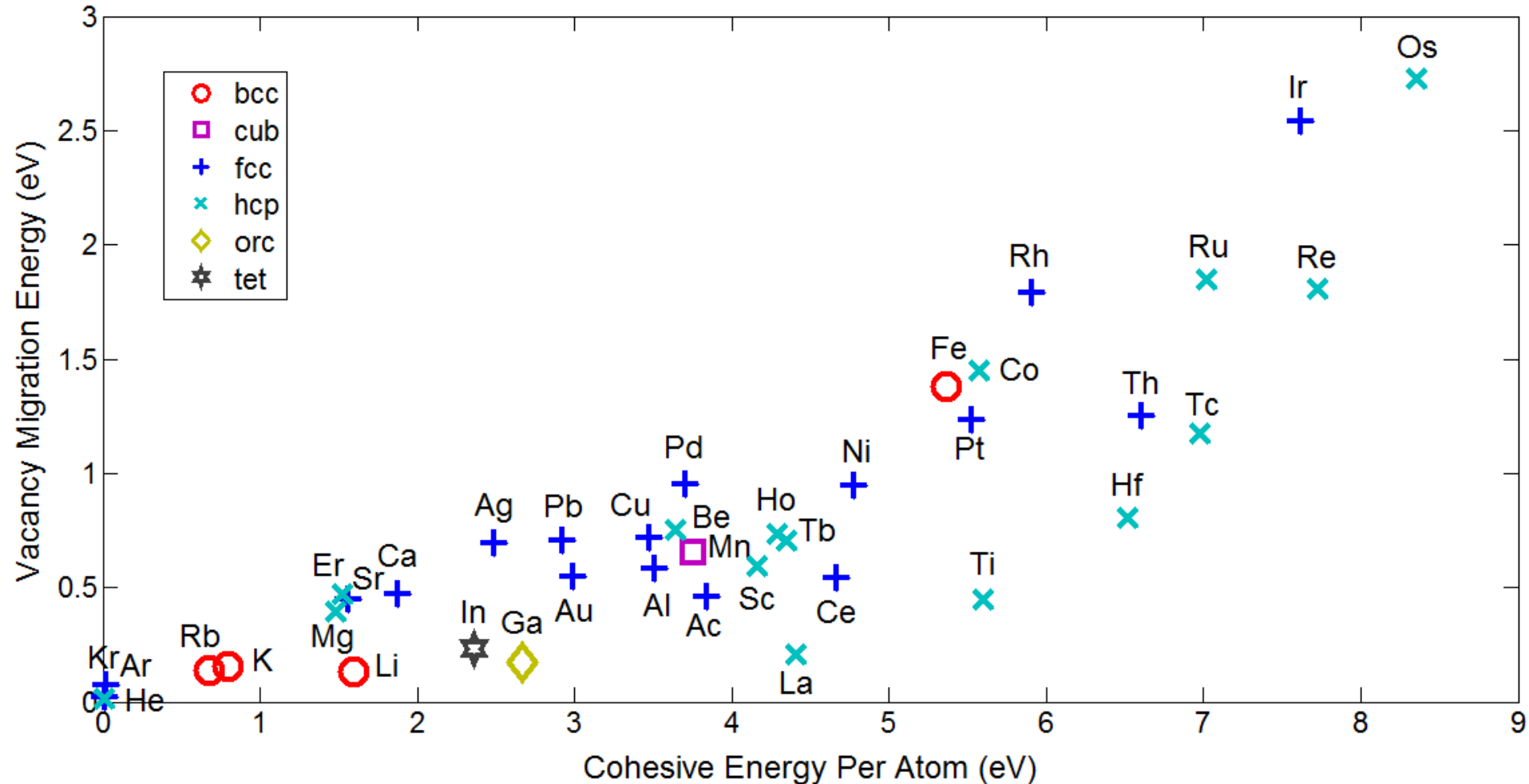


¹ A. Mattsson, et al., PRB (2002)

FCC Evac versus Ecoh/atom



FCC Emig versus Ecoh/atom



Summary of Simple Diffusion in Elements/Dilute Alloys

- High-throughput approaches can enable comprehensive databases – Large scale impact for small scale costs
 - Scale of 3 years/\$700k.
 - Addition of phonons for attempt frequencies, thermal expansion (See Chelsea Zacherl talk for efficient methods) and interstitial diffusion also practical.
- Provide critical data for CALPHAD models, trend identification.
- Have written software and are running initial database at UW.

Screening for Fast Oxygen Migration in Perovskites

Motivation

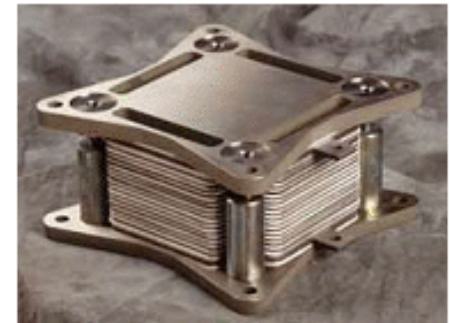
- Oxygen diffusion is important in
 - solid oxide fuel cells (esp. low T)
 - sensors (response time)
- Fast diffusion characterized by high diffusion coefficient

$$D \propto \exp\left(-\frac{E_m}{kT}\right) [V_O^{++}]$$

- Fast diffusion corresponds with low migration barrier E_m

ES-5000 Energy Server

Welcome to clean, quiet electricity that's always on. Welcome to the ES-5000 Energy Server.



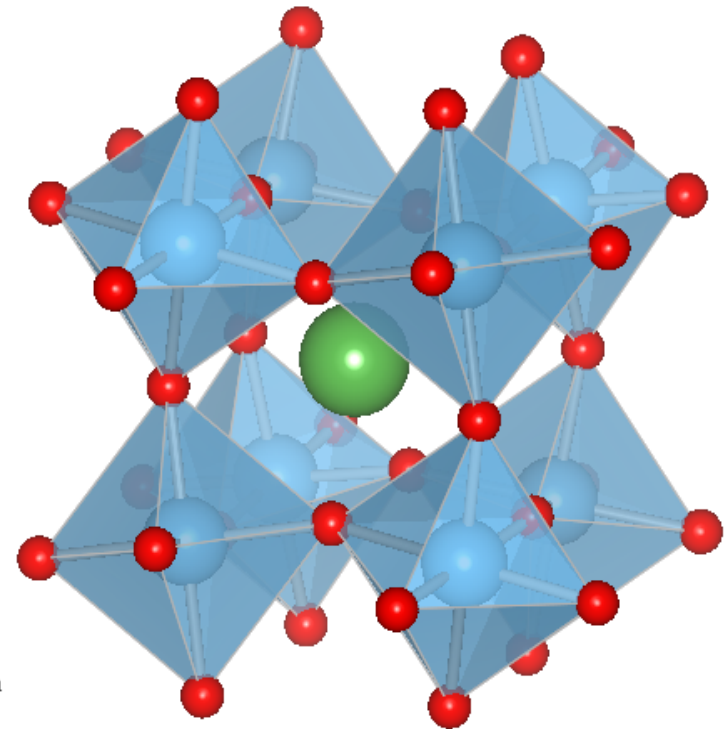
Planar SOFC - Courtesy of Siemens Westinghouse Power Corp.



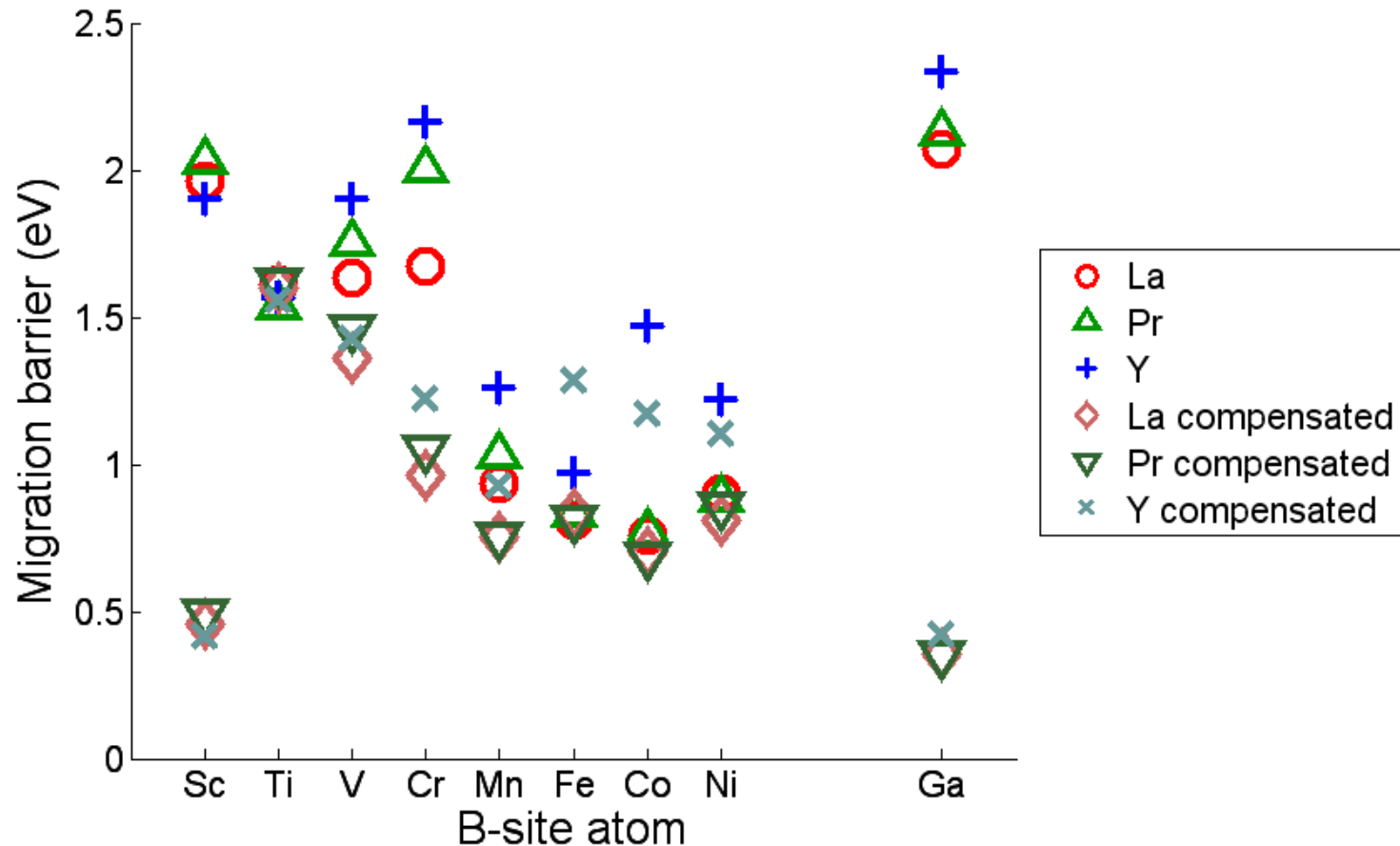
Oxygen sensor for fuel injection system
<http://www.rockauto.com>

Modeling Perovskite Oxygen Migration Barriers

- Perovskites: $A^{3+}B^{3+}O_3$
- [A = La, Pr, Y][B = 3d transition metal, Sc, Ga] O_3 = 27 systems, 54 barriers (compensated and uncompensated)
- Using VASP with PAW-GGA, PW-91, High-throughput NEB scripts
- 40-atom supercell with 4x4x4 Monkhorst-Pack kpoint mesh
- Climbing Image Nudged Elastic Band method, 3 images
- Using only one position and jump direction gives 100-200 meV error
- High-spin ferromagnetic start (high temperature operation above magnetic transition temperature)



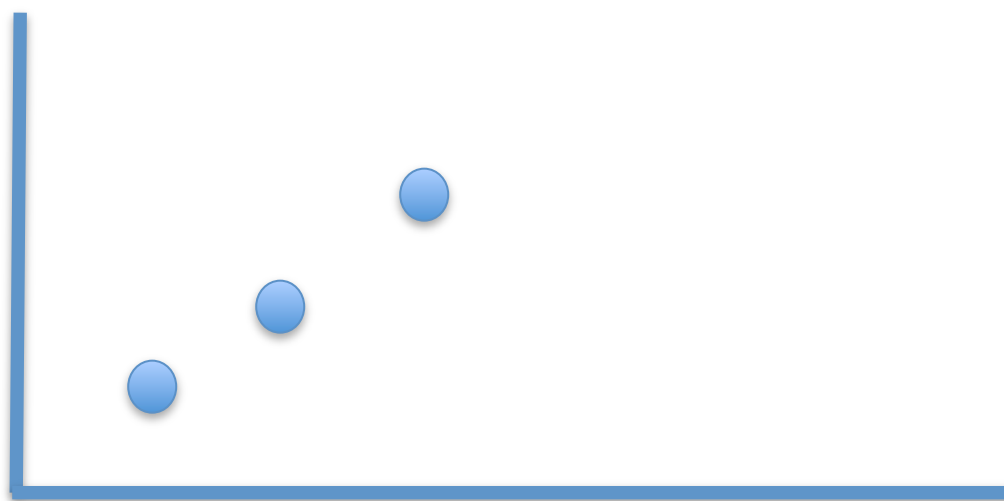
Perovskite Migration Energies



- Wide range, from 0.4-2.4 eV
- Challenging to explore whole perovskite space (>10,000 systems with A and B site alloying)
- Can we identify easy to determine descriptors to understand and predict these values?

Do Migration Barriers Trend with any Bulk or Endpoint Characteristics (Descriptors)?

Slow Calculations:
NEB-calculated
migration barrier



Fast calculations: Descriptors
derived solely from the bulk and
vacancy

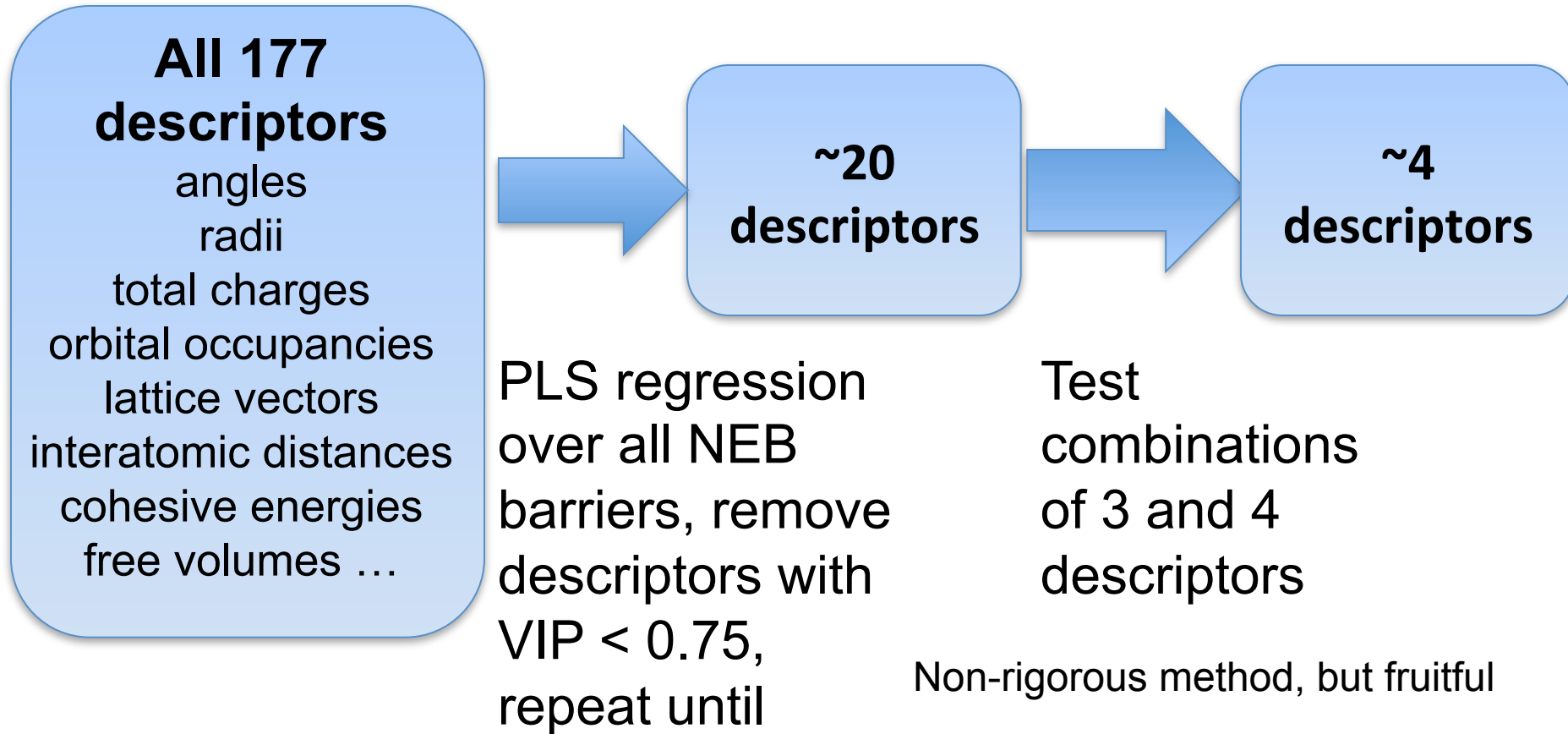
Search for Descriptors with Partial Least Squares (PLS) Regression

- PLS is a linear regression on descriptors

$$\begin{aligned} \text{PLS barrier} &= c_0 \\ &+ c_1 * (\text{value of descriptor 1}) \\ &+ c_2 * (\text{value of descriptor 2}) \\ &+ c_3 * (\text{value of descriptor 3}) + \dots \end{aligned}$$

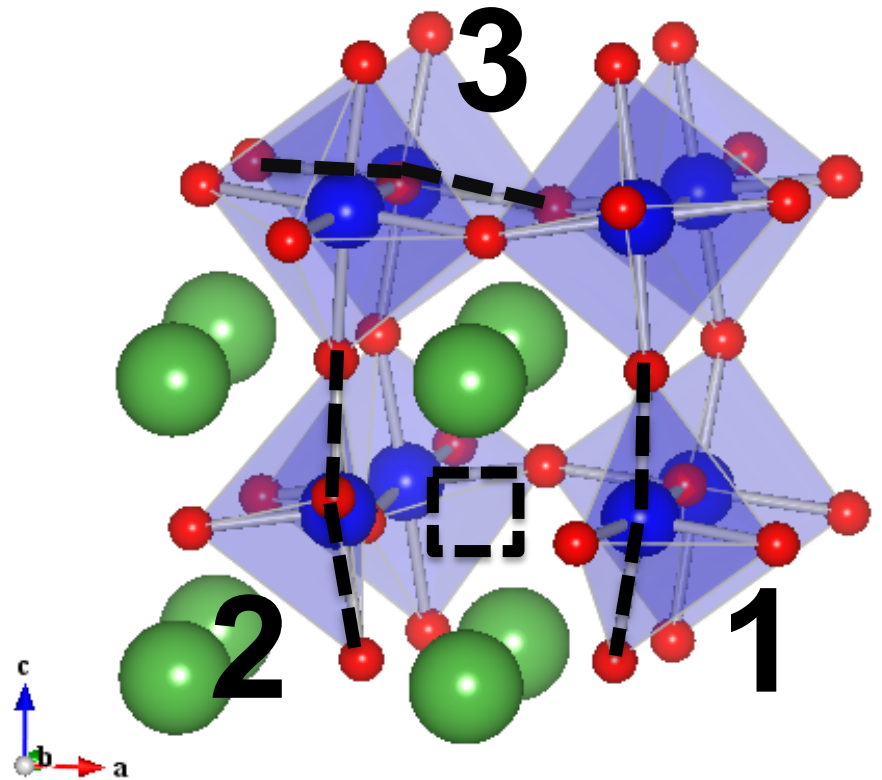
- Also returns a Variable Importance for the Projection (VIP) for each descriptor.

Choosing Descriptors

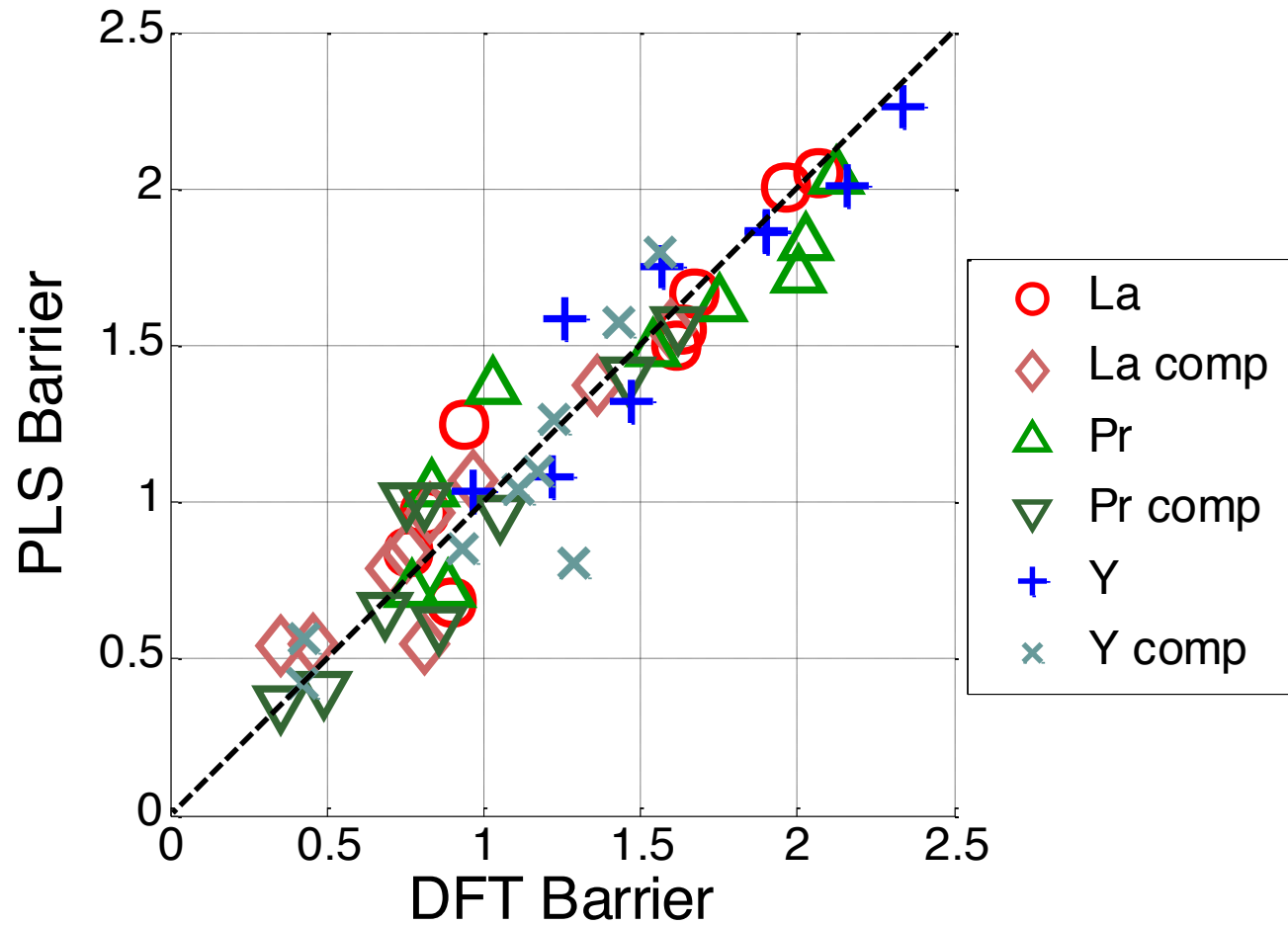


PLS Derived Descriptors

VIP	Coeff.	Description
0.00	-45.613	Intercept
1.42	0.127	O-B-O 1
1.07	-0.074	O-B-O 2
0.80	0.239	O-B-O 3
0.71	-0.030	Bulk avg. B-O-B

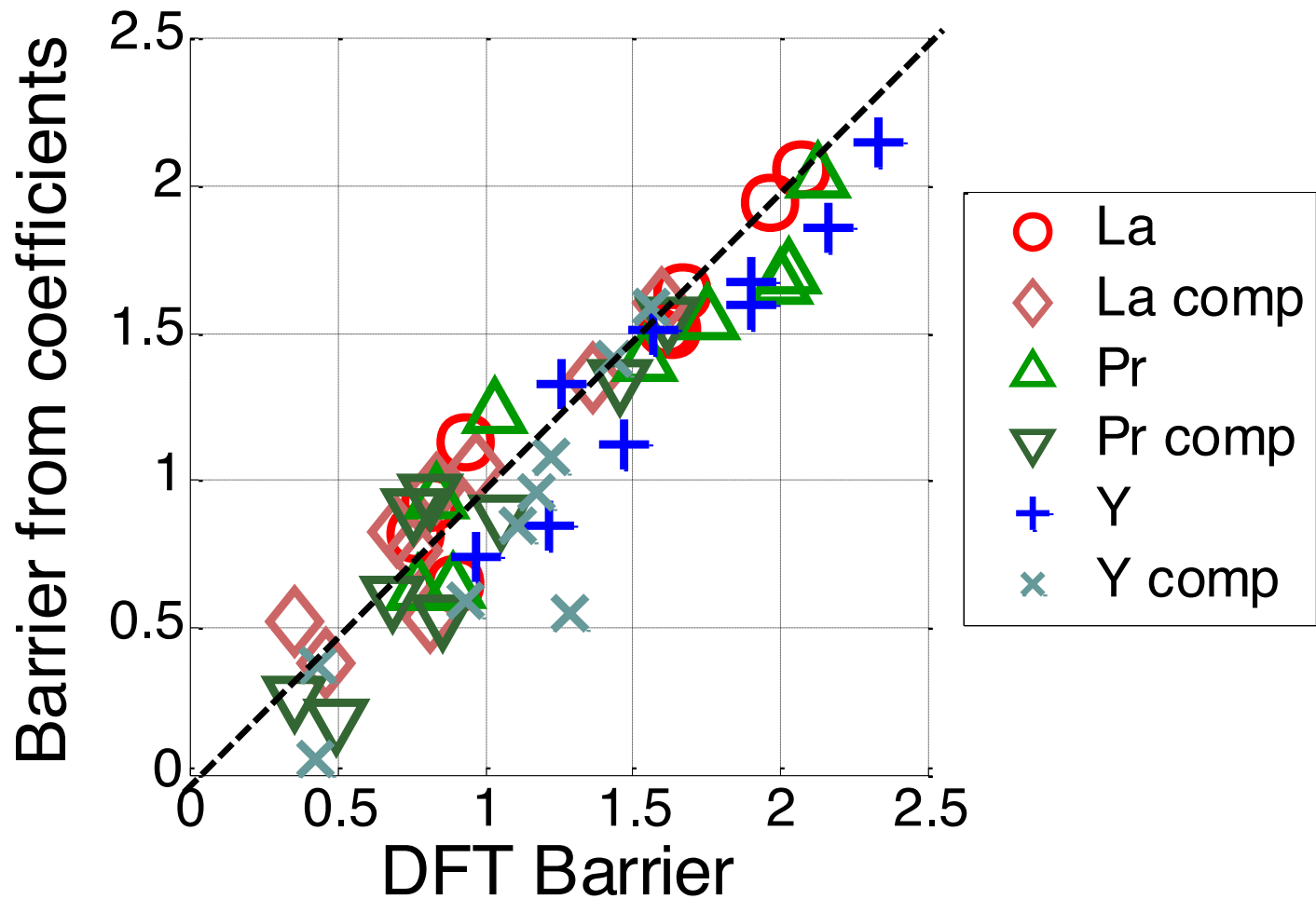


PLS Regression on All Data



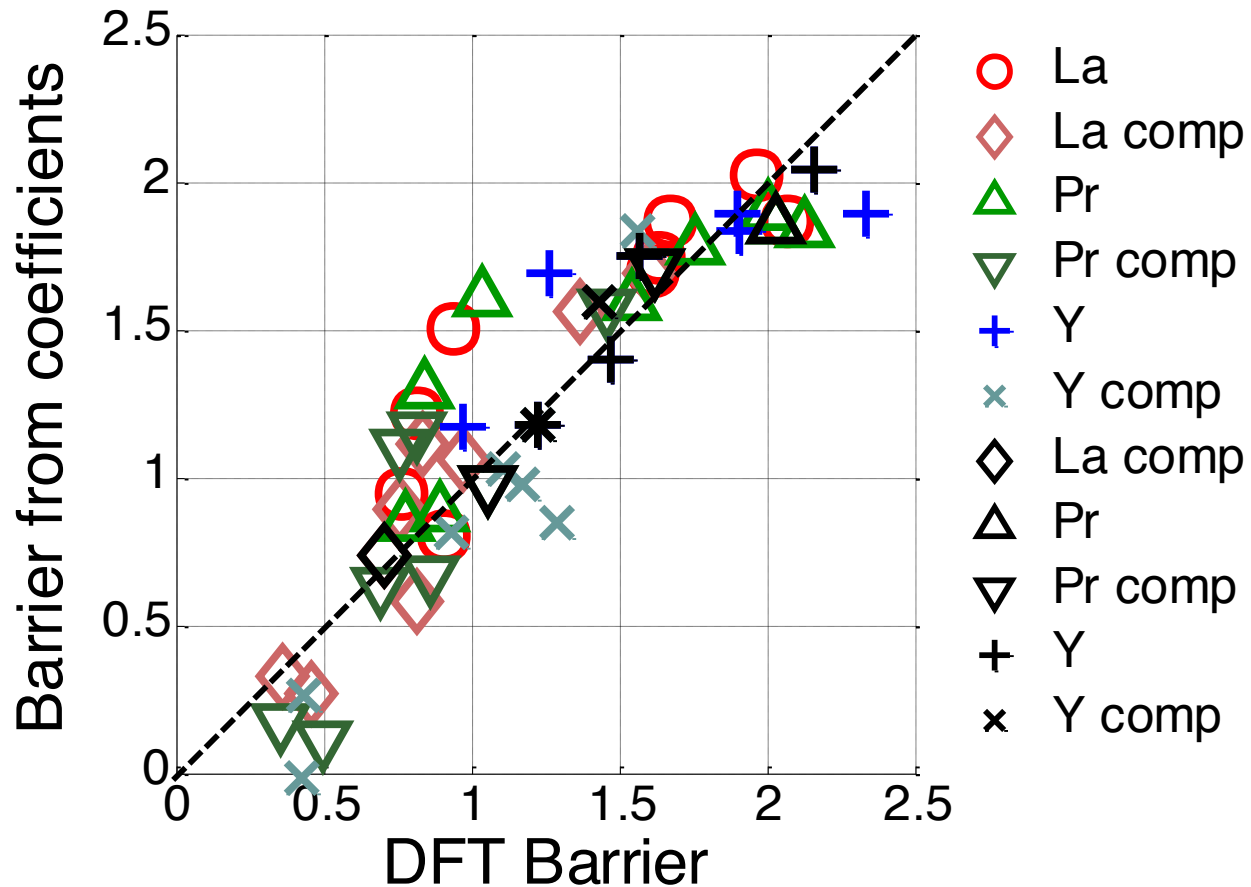
Max error: 0.50 RMS: 0.16

Predicting PrBO₃ and YBO₃ from LaBO₃



Max error: 0.73 RMS: 0.22

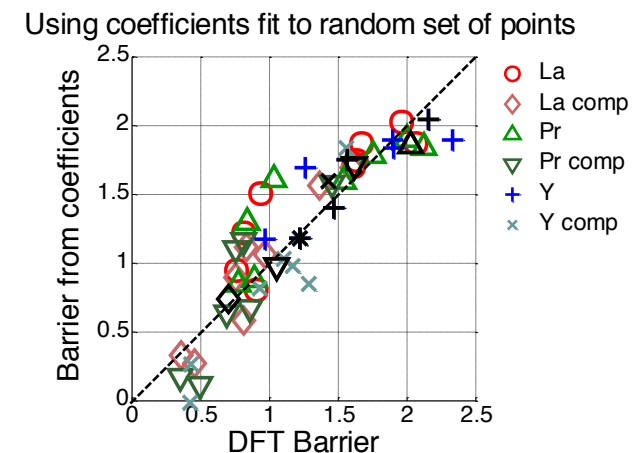
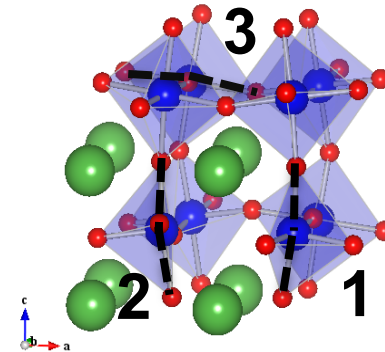
Predicting All Data from Random Subset (Fit to 10 systems)



Max error: 0.58 RMS: 0.24

Summary of Screening for Fast Oxygen Migration in Perovskites

- Migration barriers of 54 ABO_3 perovskites can be represented with only
 - three O-B-O bond angles in the first endpoint
 - the average relaxed B-O-B bond angle in the bulk in the bulk
- **Data from bulk and vacancy can now be used to screen for low barriers.**
- May be many similar ways to accelerate migration energy calculations on complex structures with **mining of descriptors**.



Ni-Cr Radiation Induced Segregation

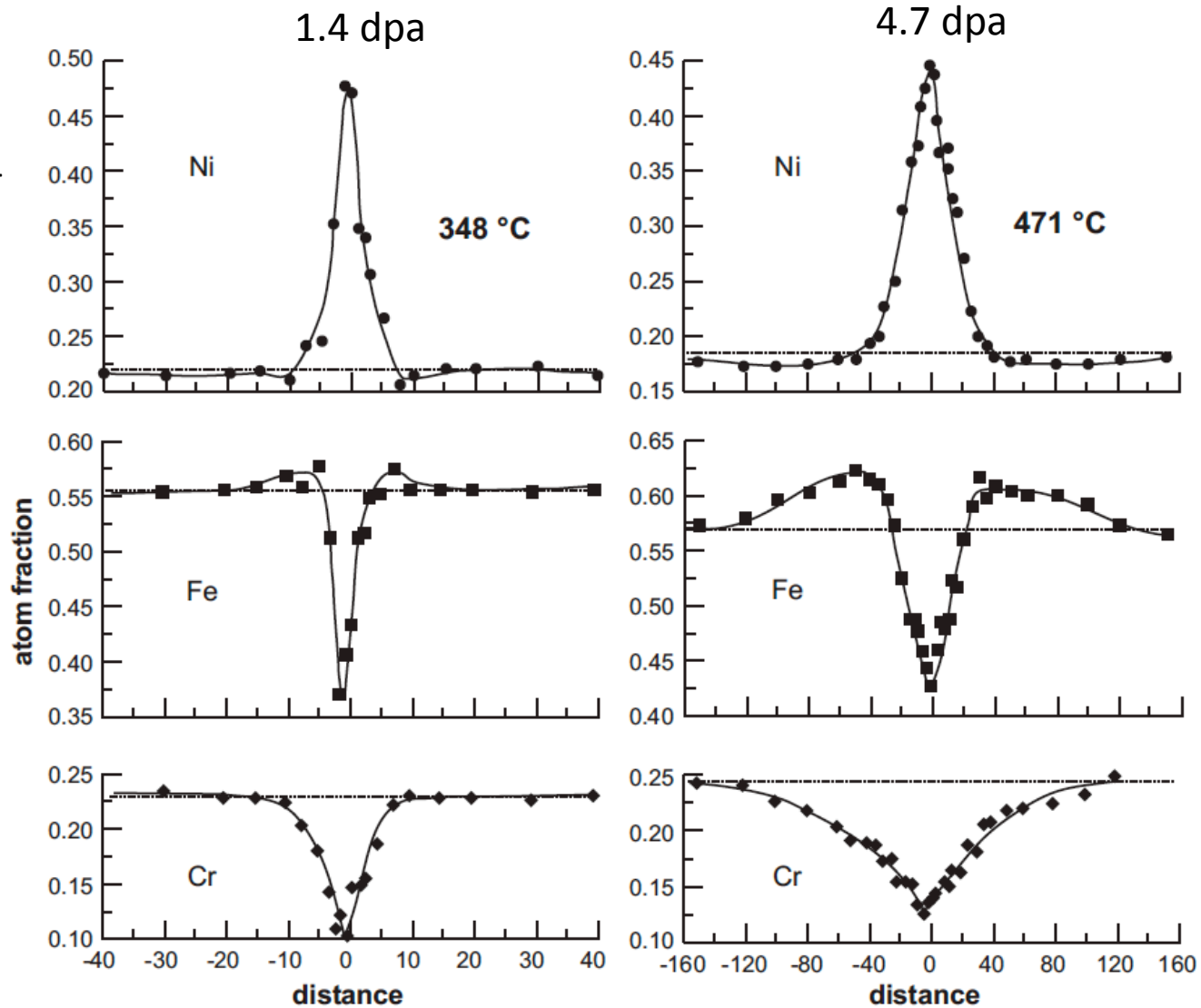
Ab initio Molecular Dynamics Approach

What is Radiation Induced Segregation (RIS)?

A change in composition at a defect sink (grain boundary, void, dislocation, surface, ...) due to unequal transport of species to the sink by radiation induced defects

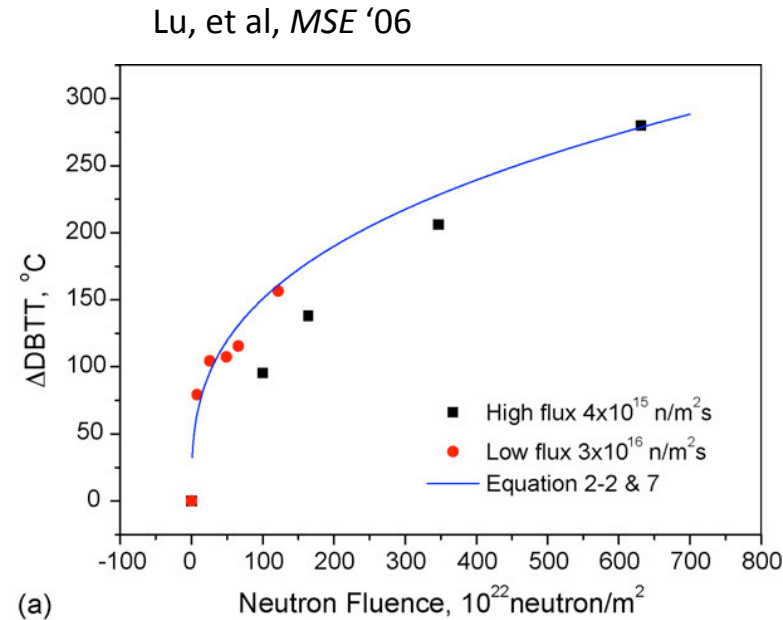
RIS in Fe-Cr-Ni Steels

Austenitic
(fcc) steel:
Fe-20Cr-25Ni-
0.8Nb (wt%)



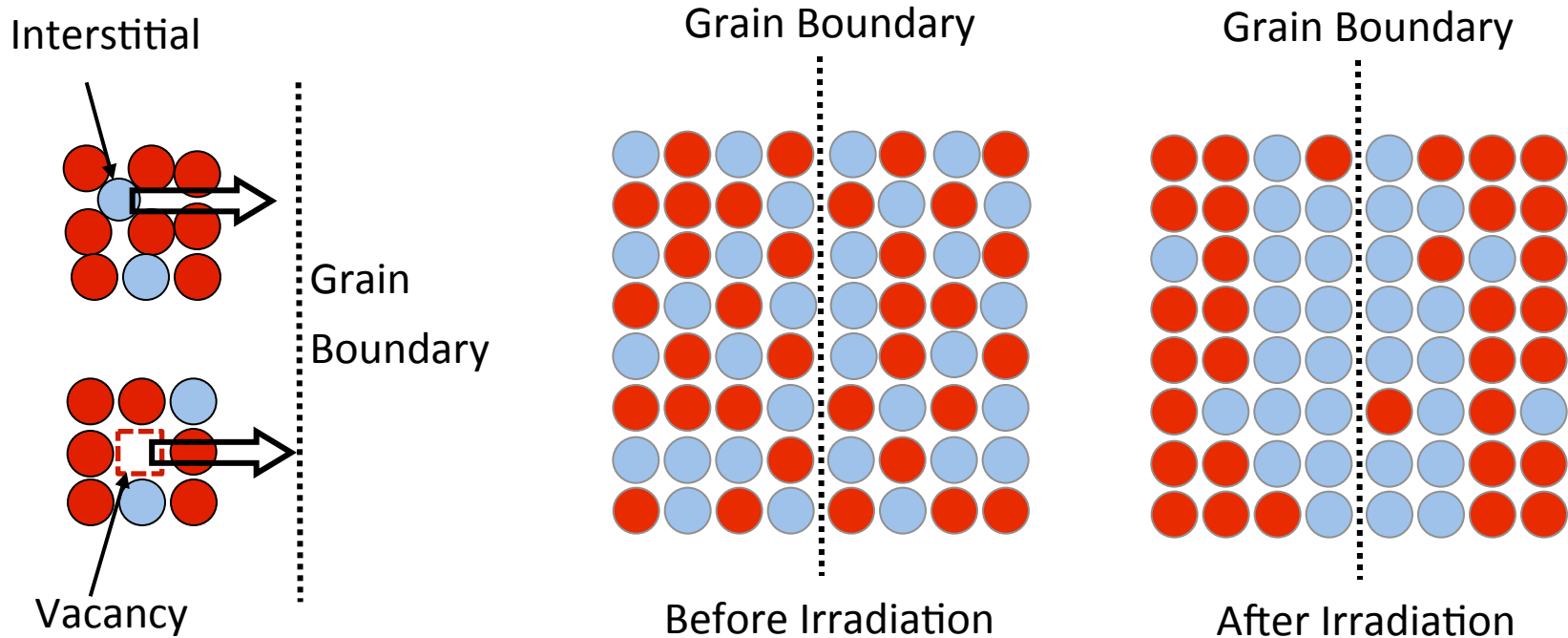
Why Does RIS Matter?

- Linked to Radiation Induced Precipitation (RIP)
- Linked with intergranular failure and void swelling
- Potentially contributes irradiation assisted stress corrosion cracking (IASCC)
- Particular interest in Cr RIS in steels as Cr is key for corrosion protection



RPV Steel DBTT due to P RIS

The Atomic Level View of RIS



Possible RIS Mechanism to Enrich Blue

- Migrates preferentially as interstitials
- Exchanges preferentially with vacancies
- Defect-solute interaction, e.g. vacancies drag species to sink

$$D_{Blue}^I > D_{Red}^I$$

$$D_{Blue}^V < D_{Red}^V$$

$$D_{VBlue} > 0$$

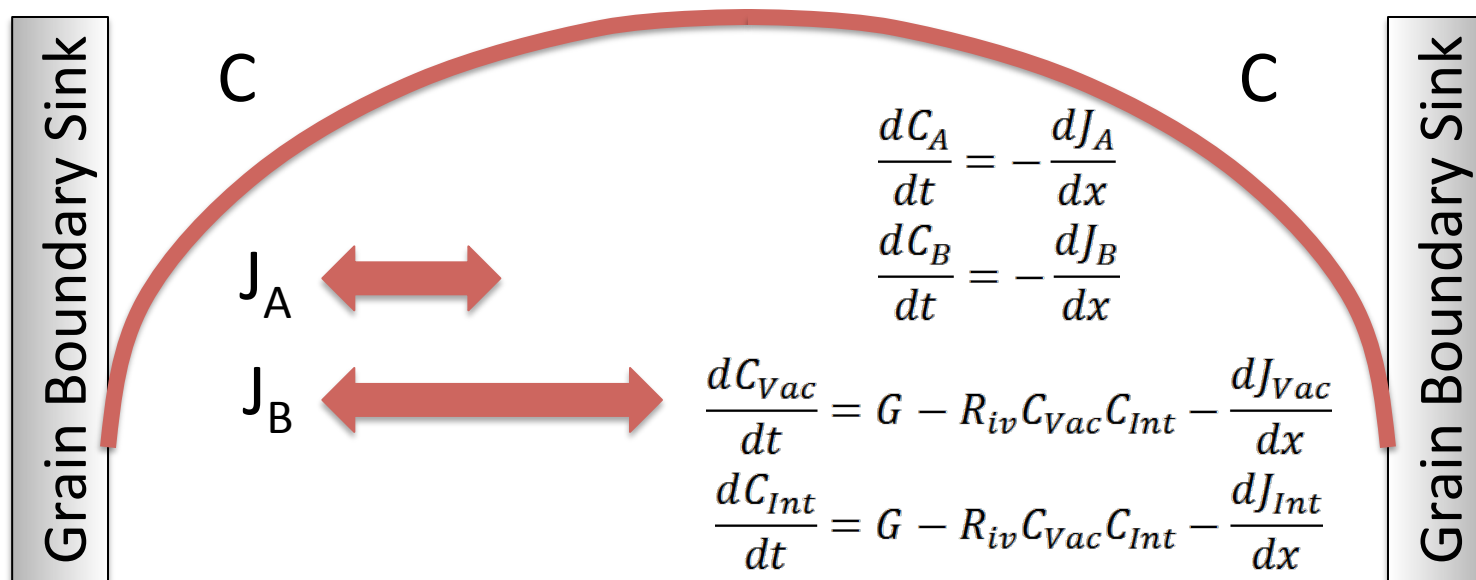
Modeling RIS

Obtain flux from diffusion coefficients

$$J_i = - \sum_{j=1}^N D_{ij} \nabla n_j$$

Wiedersich, et al., J. Nucl. Mater. '79

Solve for time evolution of concentrations with standard generation/annihilation terms and perfect sink boundary



Existing RIS Models for FCC Steels

- Many existing Cr RIS models in steels
- Mixed success in quantitative agreement on RIS prediction
- Poor qualitative agreement on mechanism
 - **Ni-solute interstitial binding:** N. Q. Lam, *Proceedings of the Symposium on Radiation Damage Analysis for Fusion Reactors* (1983)
 - **Vacancy exchange mechanism:** J.M. Perks and S.M. Murphy (BNES, London, 1987)
 - **Vacancy exchange mechanism:** S. Watanabe, et al., *J. Nucl. Mater.* (1995):
 - **Cr-Interstitial repulsion:** R.G. Faulkner, *International Workshop on Defect Production, Accumulation and Materials Performance in an Irradiation Environment* (1997)
 - **Vacancy exchange mechanism, concentrations dependent D:** T.R. Allen and G.S. Was, *Acta Materialia* (1998)
 - **Vacancy-Cr binding for TNES:** E. P. Simonen and S. M. Bruemmer (MRS Proceedings, 1999)
- **Present best model is vacancy exchange mechanism (Inverse Kirkendall)* but more fundamental understanding of active mechanisms is needed**

*G.S. Was, et al. JNM (2012)

Dilute Diffusion from Multifrequency Models

Ab Initio Energetics (E_V)



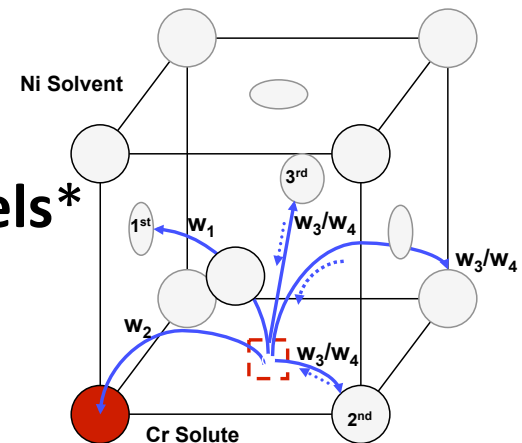
Kinetic Coefficients (D)

Thermodynamics (stat. mech. Models)
Kinetic rates (transition state theory)

Atomic scale concentrations, rates

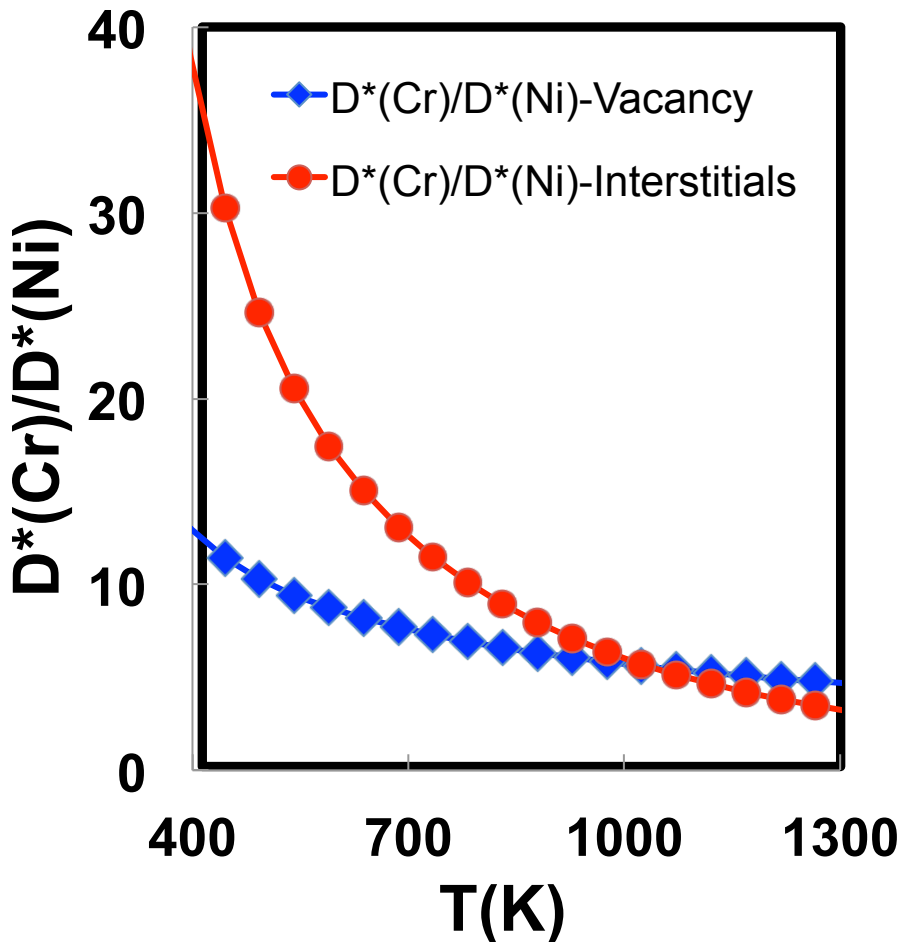
$$C_V = e^{-E_{Vf}/kT} \quad R_V = \nu e^{-E_{Vm}/kT}$$

Multifrequency models*



*A.R. Allnatt and A.B. Lidiard, *Atomic Transport in Solids*, '96

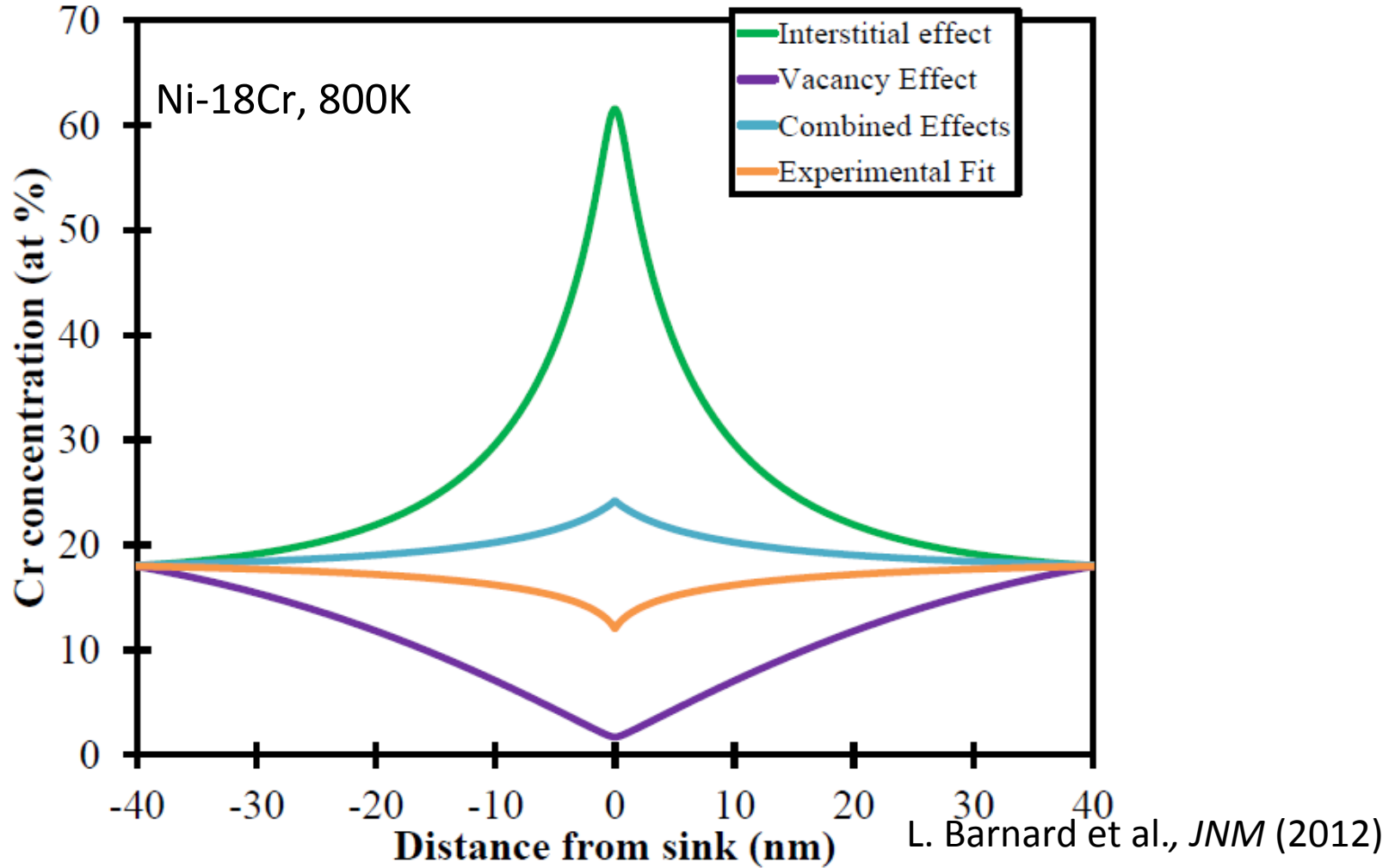
Ratio of Tracer Diffusion Coefficients



- For vacancies $D^*(Cr)/D^*(Ni) \sim 8$ (700K), typically $\sim 2-3$ from models. Cr much faster than expected!
- First insight into species dependent interstitials flux. Cr must be faster!
- Suggest new idea
 - Vacancies deplete / Interstitial enrich Cr
 - Cr RIS a balance of vacancy and interstitial contributions

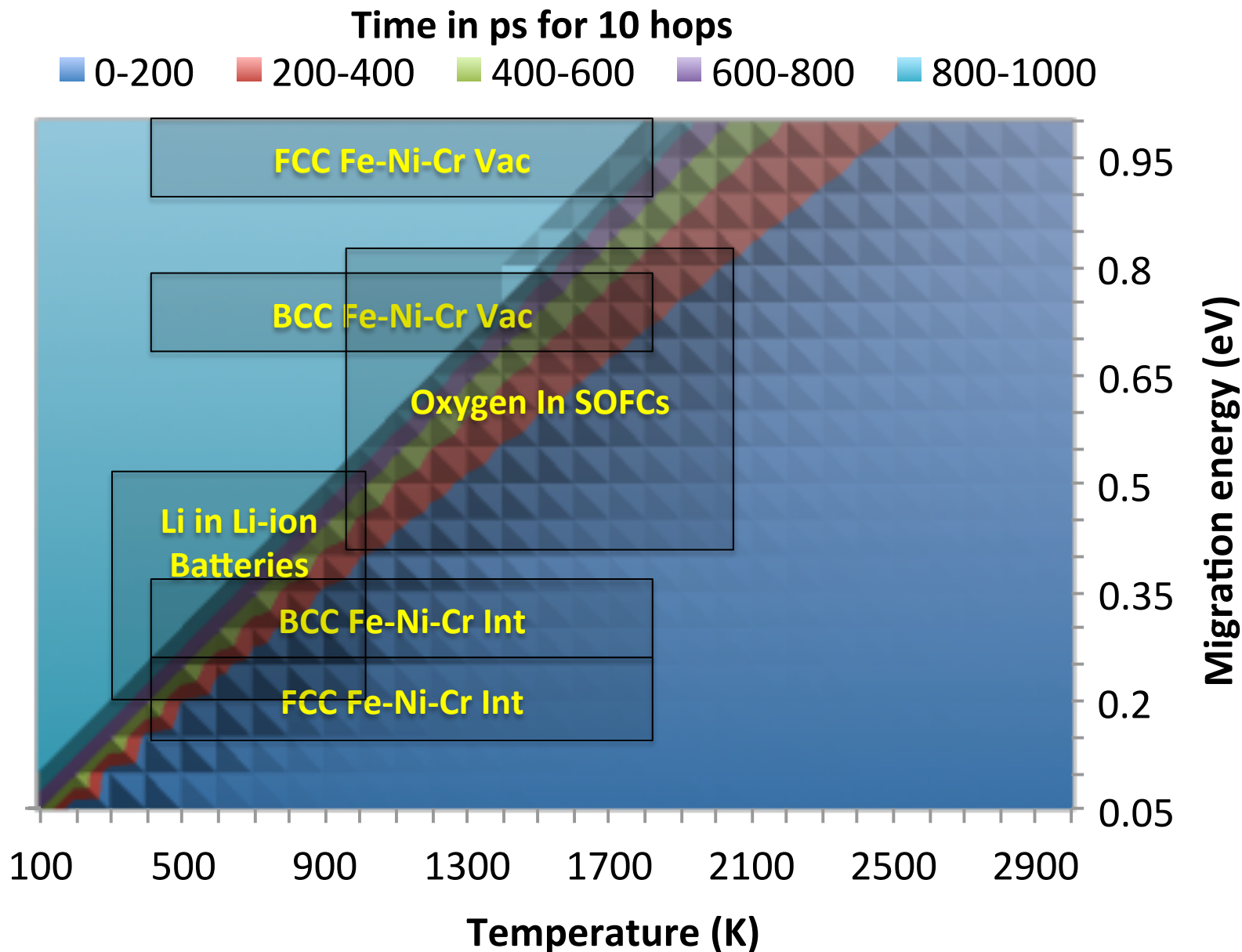
$$\Delta c_{Cr} \sim \left\{ -\frac{D_{Cr,Vac}^*}{D_{Ni,Vac}^*} + \frac{D_{Cr,Int}^*}{D_{Ni,Int}^*} \right\}$$

Interstitial vs. Vacancy Contributions to RIS

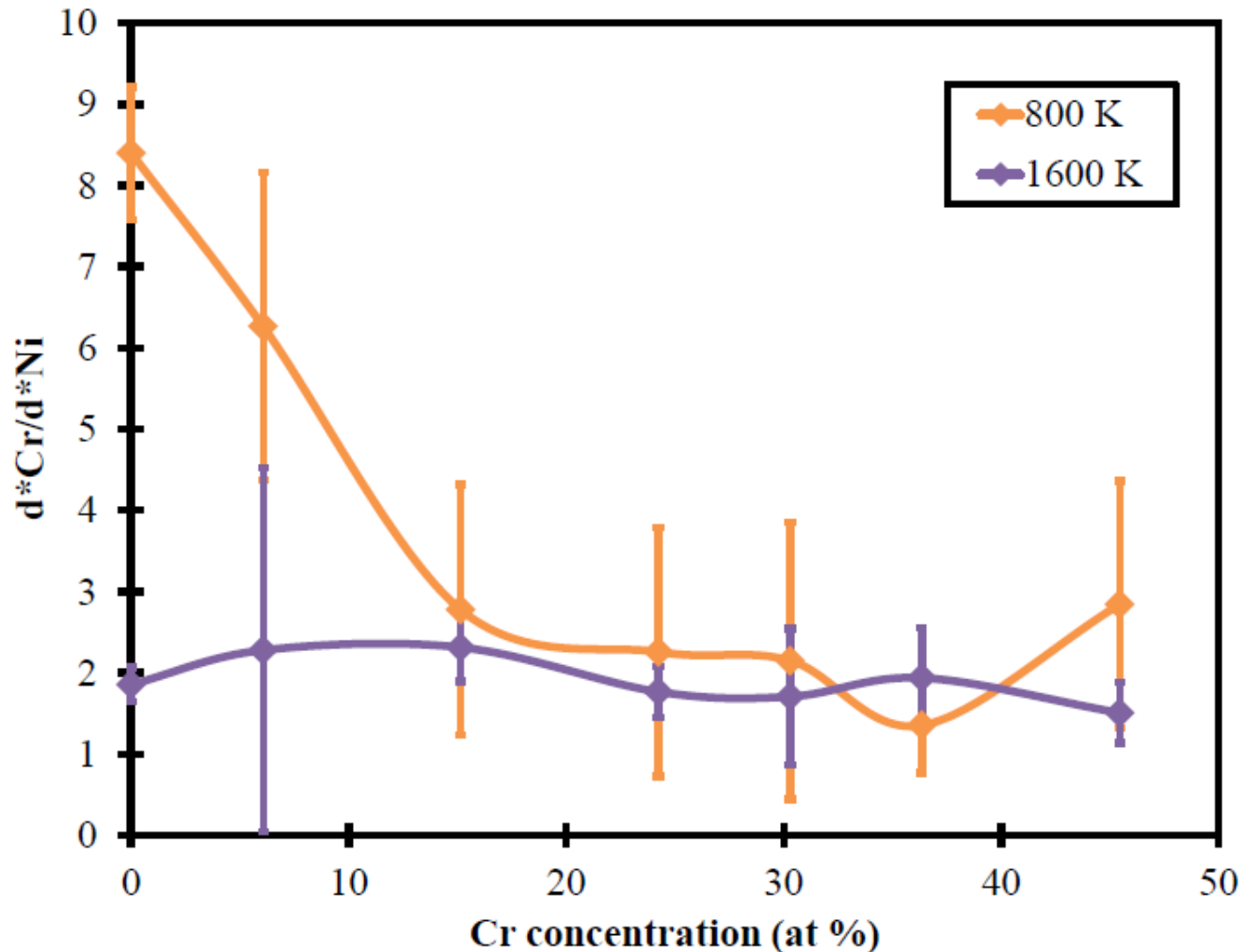


- Vacancy values consistent with experiments but too strong
- Interstitials seem to be far too strong
- Missing composition dependence of interstitials!

Systems Accessible to Ab Initio Molecular Dynamics (AIMD)

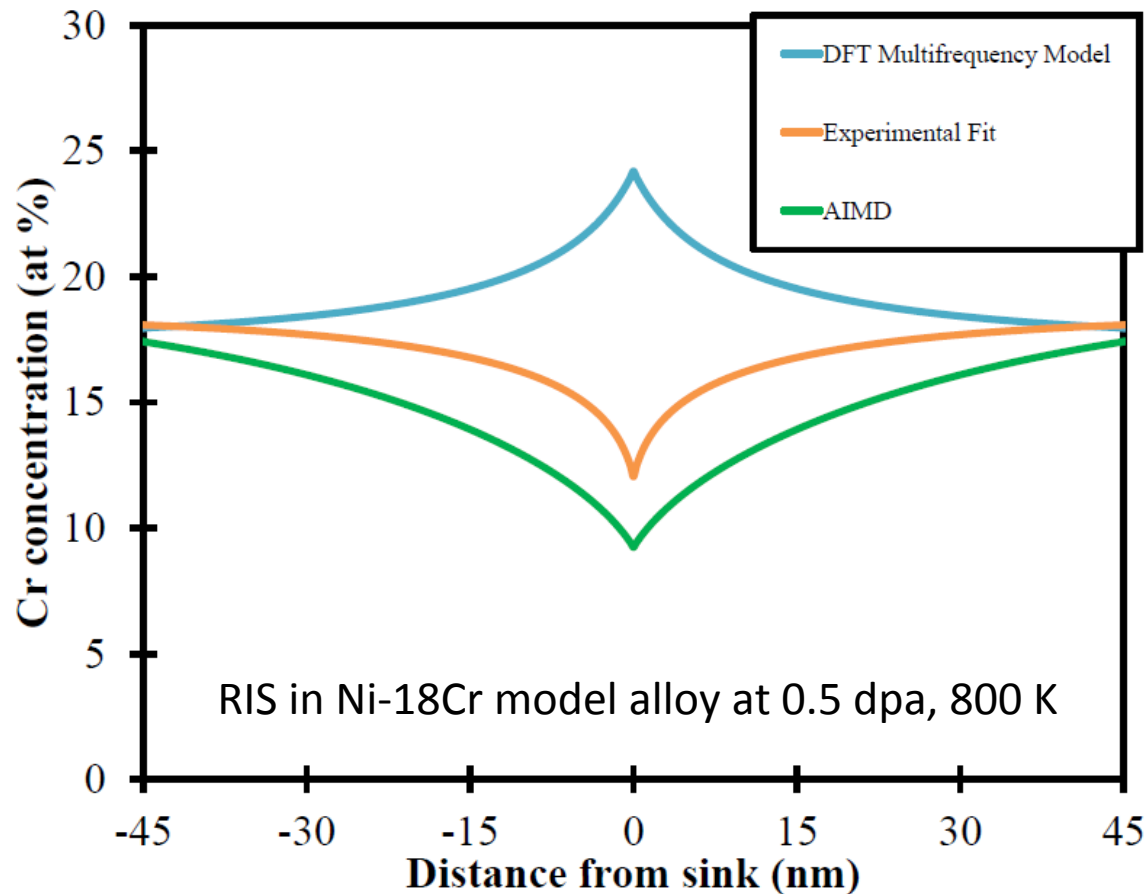


Cr and Ni Interstitial Diffusion in Ni-Cr Alloys



- Dramatic change in interstitial D_{Cr}/D_{Ni} with composition, cannot use dilute values!
- Perhaps dip seen near Ni_2Cr phase (forms experimentally at 863 K)₃₆

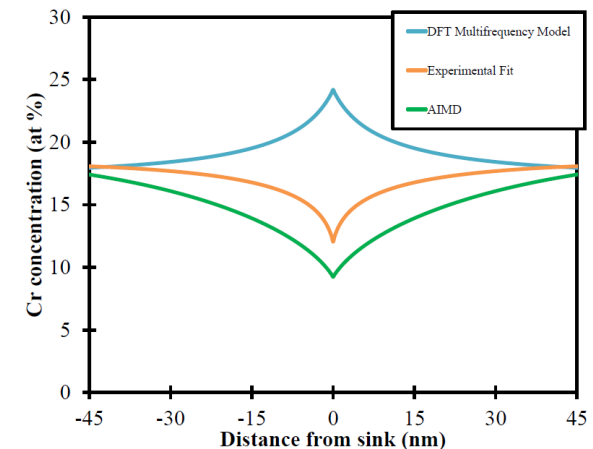
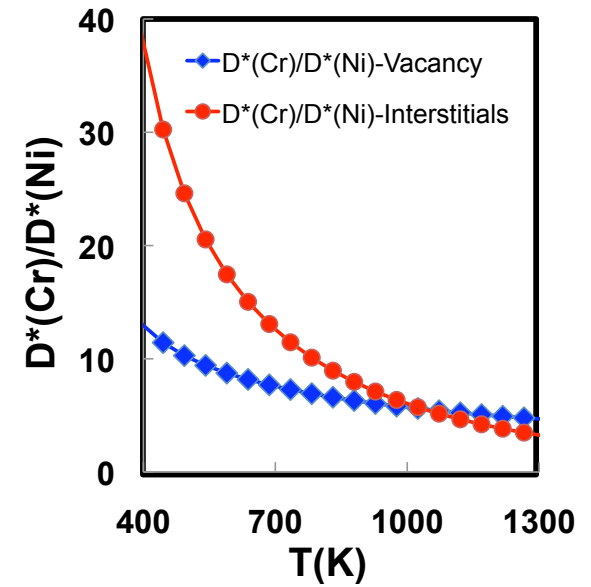
RIS Prediction from AIMD Result



- Semi-quantitative agreement with experiments.
- Validates ab initio informed model that shows coupled effect of interstitials and vacancies.
- Further fitting to experiment can yield quantitative model

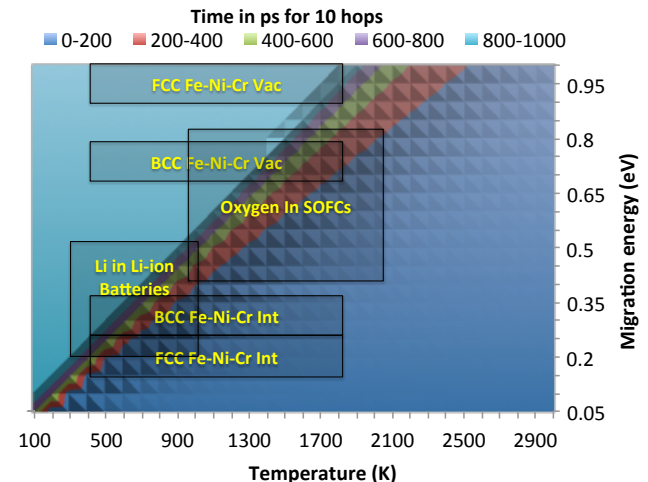
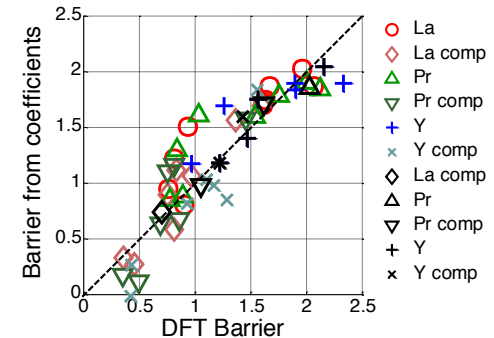
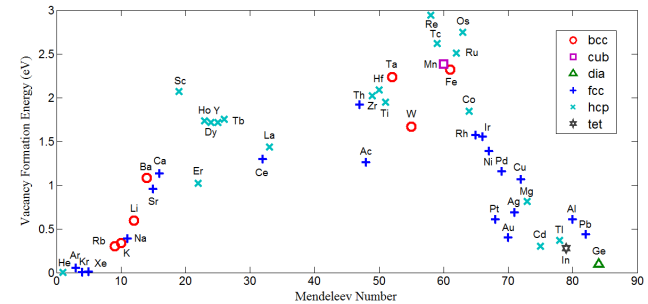
Summary of Ni-Cr RIS: Ab initio Molecular Dynamics Approach

- Ab initio based model provides **new insights** for Ni-Cr RIS
 - Vacancy mechanism: Cr much faster than Ni than previously thought.
 - Interstitial mechanism: Strong interstitial bias for Cr over Ni – not previously included in any model.
 - **Observed Cr RIS in steels likely a balance of strong interstitial and vacancy RIS tendencies**
- Concentration dependent diffusion coefficients obtained from ab initio molecular dynamics – powerful tool for low-barrier systems ($\sim 0.5\text{eV}$)



Overall Summary

- **High-throughput** ab initio simulations can provide massive diffusion coefficient databases at fraction of the cost of experiment
 - DFT accuracy an issue
 - Level of detail of simulation (attempt frequencies, G_{mig} vs. E_{mig})
- Diffusion in simple systems is now accessible to **high-throughput and datamining approaches**
 - Database of E_{vac} , E_{mig} in dilute alloys in standard structures (3 years/\$700k)
 - Perovskites – predicting of E_{mig} with just 4 descriptors can speed searches
- Diffusion in alloys amenable to **direct ab initio MD** for low barrier systems $\sim(0.5$ eV)
 - Demonstrated semi-quantitative model for RIS
 - Could enable straightforward database development with enough computing time



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* Leland Bernard * Maneesh Mishra
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* Ryan Jacobs * Shenzen Xu
* Tam Mayeshiba * Wei Xie
* Xing Wang * Yun Liu
* Zhizhang Shen

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* Jing Han * Jianhong Dai

Undergraduate student

* Tom Angsten

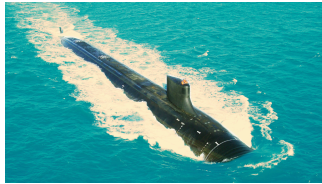


<http://matmodel.engr.wisc.edu/>

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Herb Endowment for Physics

XSEDE

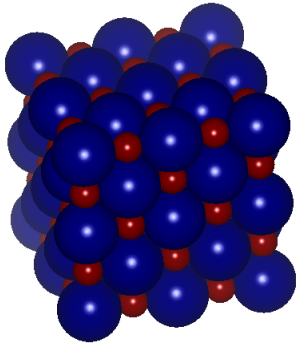
Extreme Science and Engineering
Discovery Environment

Computing time provided by
NSF TG-DMR110074 and
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Backup Slides

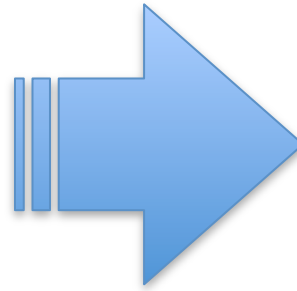
Integrating with Other Tools

Perform job-specific functions



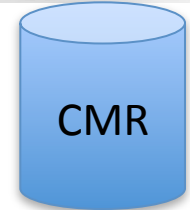
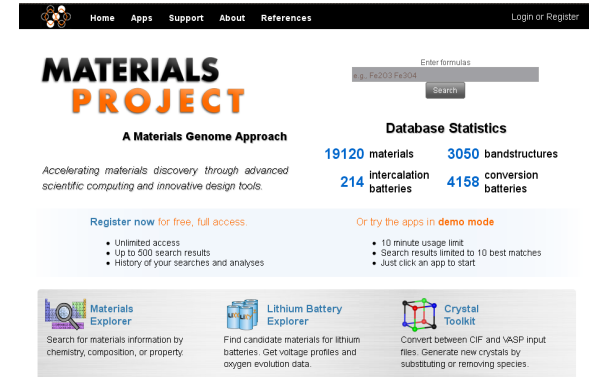
- Use ASE¹, aconvasp², or other code to:
- Generate crystal structures
 - View and manipulate supercells
 - Interpolate NEB images
 - Extract and compare energies

Manage sequence of jobs



- Use our code to:
- Queue jobs
 - Monitor jobs
 - Call job-specific functions as needed
 - Advance job sequence
 - Restart unfinished sequence at any step

Obtain and store migration barriers and VFEs



Integrate results with another database project (Materials Project)³ or present them in a common format (Computational Materials Repository)⁴

¹Atomic Simulation Environment: S. R. Bahn and K. W. Jacobsen, *Comput. Sci. Eng.* (2002); ²S. Curtarolo, et al., *Comp. Mat. Sci.* (2012); ³<http://www.materialsproject.org/>; ⁴<https://wiki.fysik.dtu.dk/ase/>, Computational Materials Repository at <https://wiki.fysik.dtu.dk/cmnr/>

FCC Status 4/16/12

<http://www.periodni.com>

PERIOD	GROUP																													
	1 IA	2 IIA	3	4	5	6	7	8	9	10	11	12	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA												
1	1 1.0079 H HYDROGEN												5 10.811 B BORON	6 12.011 C CARBON	7 14.007 N NITROGEN	8 15.999 O OXYGEN	9 18.998 F FLUORINE	10 20.180 Ne NEON	18 4.0026 He HELIUM											
2	3 6.941 Li LITHIUM	4 9.0122 Be BERYLLIUM											13 26.982 Al ALUMINUM	14 28.086 Si SILICON	15 30.974 P PHOSPHORUS	16 32.065 S SULPHUR	17 35.453 Cl CHLORINE	18 39.948 Ar ARGON												
3	11 22.990 Na SODIUM	12 24.305 Mg MAGNESIUM											19 39.098 K POTASSIUM	20 40.078 Ca CALCIUM	21 44.956 Sc SCANDIUM	22 47.887 Ti TITANIUM	23 50.942 V VANADIUM	24 51.996 Cr CHROMIUM	25 54.938 Mn MANGANESE	26 55.845 Fe IRON	27 58.933 Co COBALT	28 58.693 Ni NICKEL	29 63.546 Cu COPPER	30 65.38 Zn ZINC	31 69.723 Ga GALLIUM	32 72.64 Ge GERMANIUM	33 74.922 As ARSENIC	34 78.96 Se SELENIUM	35 79.904 Br BROMINE	36 83.798 Kr KRYPTON
4	37 85.468 Rb RUBIDIUM	38 87.62 Sr STRONTIUM	39 88.906 Y YTTRIUM	40 91.224 Zr ZIRCONIUM	41 92.906 Nb NIOBIUM	42 95.96 Mo MOLYBDENUM	43 (98) Tc TECHNETIUM	44 101.07 Ru RUTHENIUM	45 102.91 Rh RHODIUM	46 106.42 Pd PALLADIUM	47 107.87 Ag SILVER	48 112.41 Cd CADMIUM	49 114.82 In INDIUM	50 118.71 Sn TIN	51 121.76 Sb ANTIMONY	52 127.60 Te TELLURIUM	53 126.90 I IODINE	54 131.29 Xe XENON												
5	55 132.91 Cs CAESIUM	56 137.33 Ba BARIUM	57-71 La-Lu Lanthanide	72 178.49 Hf HAFNIUM	73 180.95 Ta TANTALUM	74 183.84 W TUNGSTEN	75 186.21 Re RHENIUM	76 190.23 Os OSMIUM	77 192.22 Ir IRIDIUM	78 195.08 Pt PLATINUM	79 196.97 Au GOLD	80 200.59 Hg MERCURY	81 204.38 Tl THALLIUM	82 207.2 Pb LEAD	83 208.98 Bi BISMUTH	84 (209) Po POLONIUM	85 (210) At ASTATINE	86 (222) Rn RADON												
6	87 (223) Fr FRANCIUM	88 (226) Ra RADIUM	89-103 Ac-Lr Actinide	104 (267) Rf RUTHERFORDIUM	105 (268) Db DUBNIUM	106 (271) Sg SEABORGIUM	107 (272) Bh BOHRIUM	108 (277) Hs HASSIUM	109 (276) Mt MEITNERIUM	110 (281) Ds DARWSTADIUM	111 (280) Rg ROENTGENIUM	112 (285) Cn COPERNICIUM																		

- complete
- running
- failed
- omitted

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LANTHANIDE														
57 138.91 La LANTHANUM	58 140.12 Ce CERIUM	59 140.91 Pr PRASEODYMIUM	60 144.24 Nd NEODYMIUM	61 (145) Pm PROMETHIUM	62 150.36 Sm SAMARIUM	63 151.96 Eu EUROPIUM	64 157.25 Gd GADOLINIUM	65 158.93 Tb TERBIUM	66 162.50 Dy DYSPROSIUM	67 164.93 Ho HOLMIUM	68 167.26 Er ERBIUM	69 168.93 Tm THULIUM	70 173.05 Yb YTTERIUM	71 174.97 Lu LUTETIUM

ACTINIDE														
89 (227) Ac ACTINIUM	90 232.04 Th THORIUM	91 231.04 Pa PROTACTINIUM	92 238.03 U URANIUM	93 (237) Np NEPTUNIUM	94 (244) Pu PLUTONIUM	95 (243) Am AMERICIUM	96 (247) Cm CURIUM	97 (247) Bk BERKELIUM	98 (251) Cf CALIFORNIUM	99 (252) Es EINSTEINIUM	100 (257) Fm FERMIUM	101 (258) Md MEDELEVIUM	102 (259) No NOBELIUM	103 (262) Lr LAWRENCIUM

HCP Status 4/16/12

<http://www.periodni.com>

PERIOD	GROUP 1 IA		GROUP 2 IIA		TRANSITION METALS										GROUPS 13-18					
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
1	H 1.0079 HYDROGEN																		He 4.0026 HELIUM	
2	Li 6.941 LITHIUM	Be 9.0122 BERYLLIUM											B 10.811 BORON	C 12.011 CARBON	N 14.007 NITROGEN	O 15.999 OXYGEN	F 18.998 FLUORINE	Ne 20.180 NEON		
3	Na 22.990 SODIUM	Mg 24.305 MAGNESIUM											Al 26.982 ALUMINUM	Si 28.086 SILICON	P 30.974 PHOSPHORUS	S 32.065 SULPHUR	Cl 35.453 CHLORINE	Ar 39.948 ARGON		
4	K 39.098 POTASSIUM	Ca 40.078 CALCIUM	Sc 44.956 SCANDIUM	Ti 47.867 TITANIUM	V 50.942 VANADIUM	Cr 51.996 CHROMIUM	Mn 54.938 MANGANESE	Fe 55.845 IRON	Co 58.933 COBALT	Ni 58.693 NICKEL	Cu 63.546 COPPER	Zn 65.38 ZINC	Ga 69.723 GALLIUM	Ge 72.64 GERMANIUM	As 74.922 ARSENIC	Se 78.96 SELENIUM	Br 79.904 BROMINE	Kr 83.798 KRYPTON		
5	Rb 85.468 RUBIDIUM	Sr 87.62 STRONTIUM	Y 88.906 YTTRIUM	Zr 91.224 ZIRCONIUM	Nb 92.906 NIOBIUM	Mo 95.96 MOLYBDENUM	Tc (98) TECHNETIUM	Ru 101.07 RUTHENIUM	Rh 102.91 RHODIUM	Pd 106.42 PALLADIUM	Ag 107.87 SILVER	Cd 112.41 CADMIUM	In 114.82 INDIUM	Sn 118.71 TIN	Sb 121.76 ANTIMONY	Te 127.60 TELLURIUM	I 126.90 IODINE	Xe 131.29 XENON		
6	Cs 132.91 CAESIUM	Ba 137.33 BARIUM	La-Lu 57-71 Lanthanide	Hf 178.49 HAFNIUM	Ta 180.95 TANTALUM	W 183.84 TUNGSTEN	Re 186.21 RHENIUM	Os 190.23 OSMIUM	Ir 192.22 IRIDIUM	Pt 195.08 PLATINUM	Au 196.97 GOLD	Hg 200.59 MERCURY	Tl 204.38 THALLIUM	Pb 207.2 LEAD	Bi 208.98 BISMUTH	Po (209) POLONIUM	At (210) ASTATINE	Rn (222) RADON		
7	Fr (223) FRANCIUM	Ra (226) RADIUM	Ac-Lr 89-103 Actinide	Rf (267) RUTHERFORDIUM	Db (268) DUBNIUM	Sg (271) SEABORGIUM	Bh (272) BOHRIUM	Hs (277) HASSIUM	Mt (276) MEITNERIUM	Ds (281) DARWSTADIUM	Rg (280) ROENTGENIUM	Cn (285) COPERNICIUM								

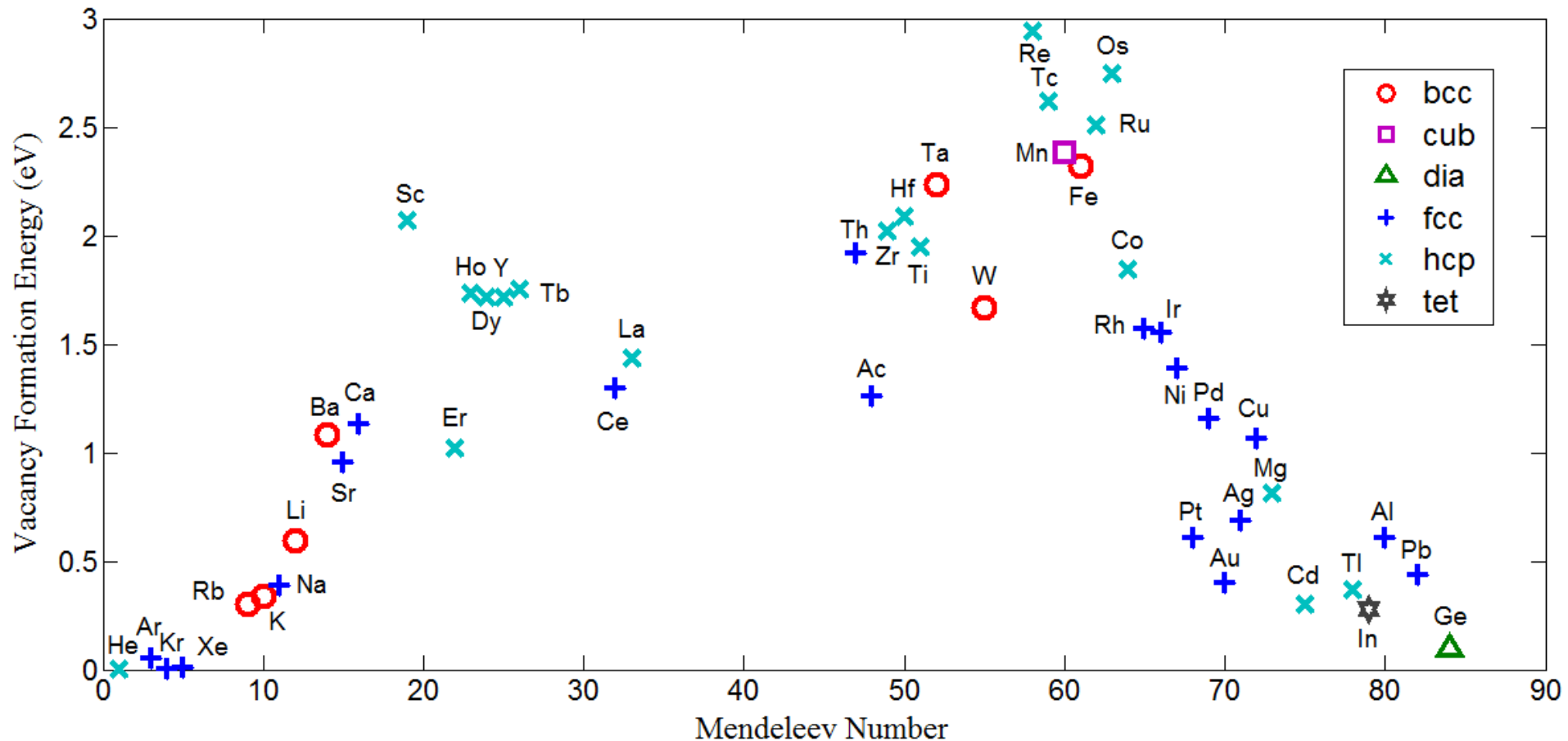
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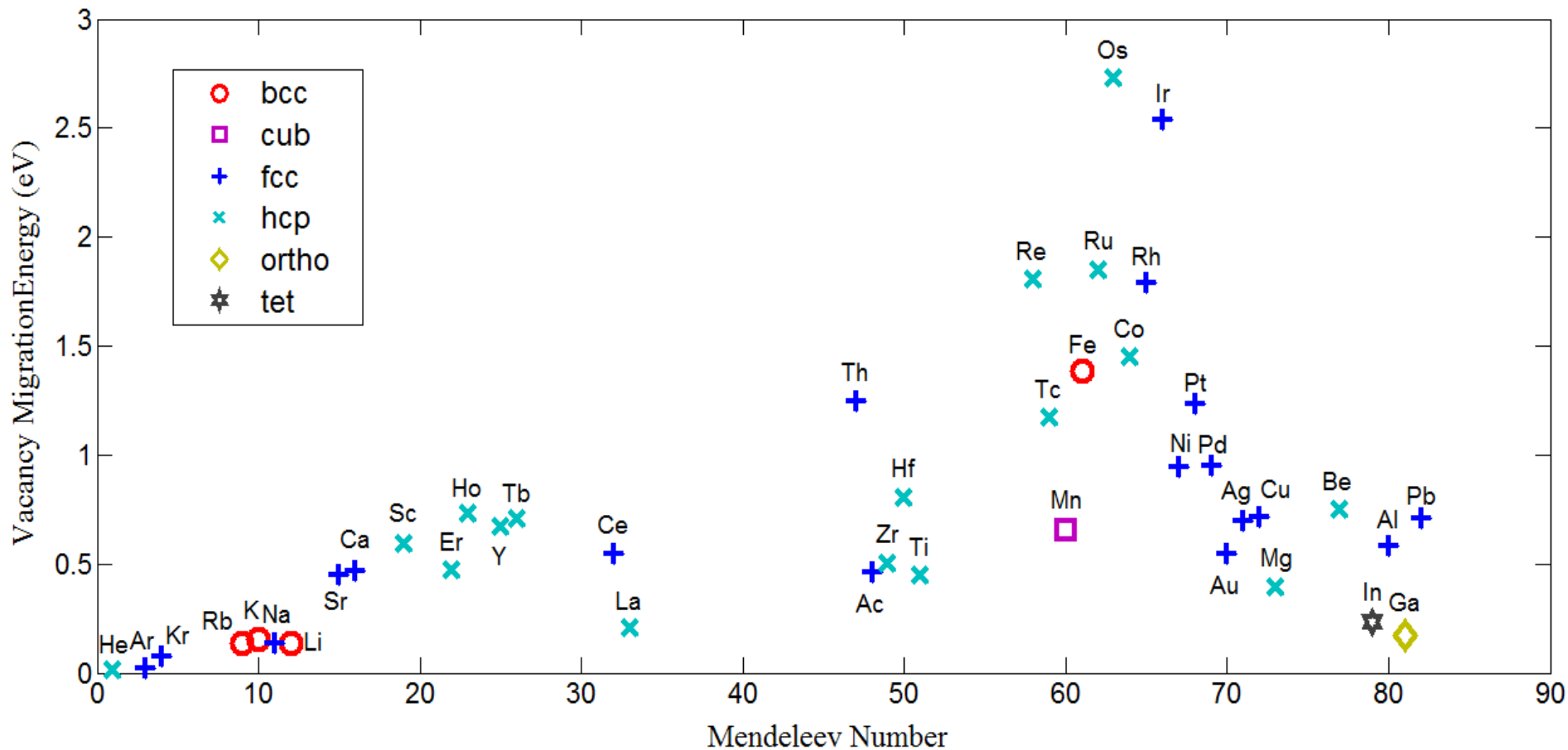
LANTHANIDE														
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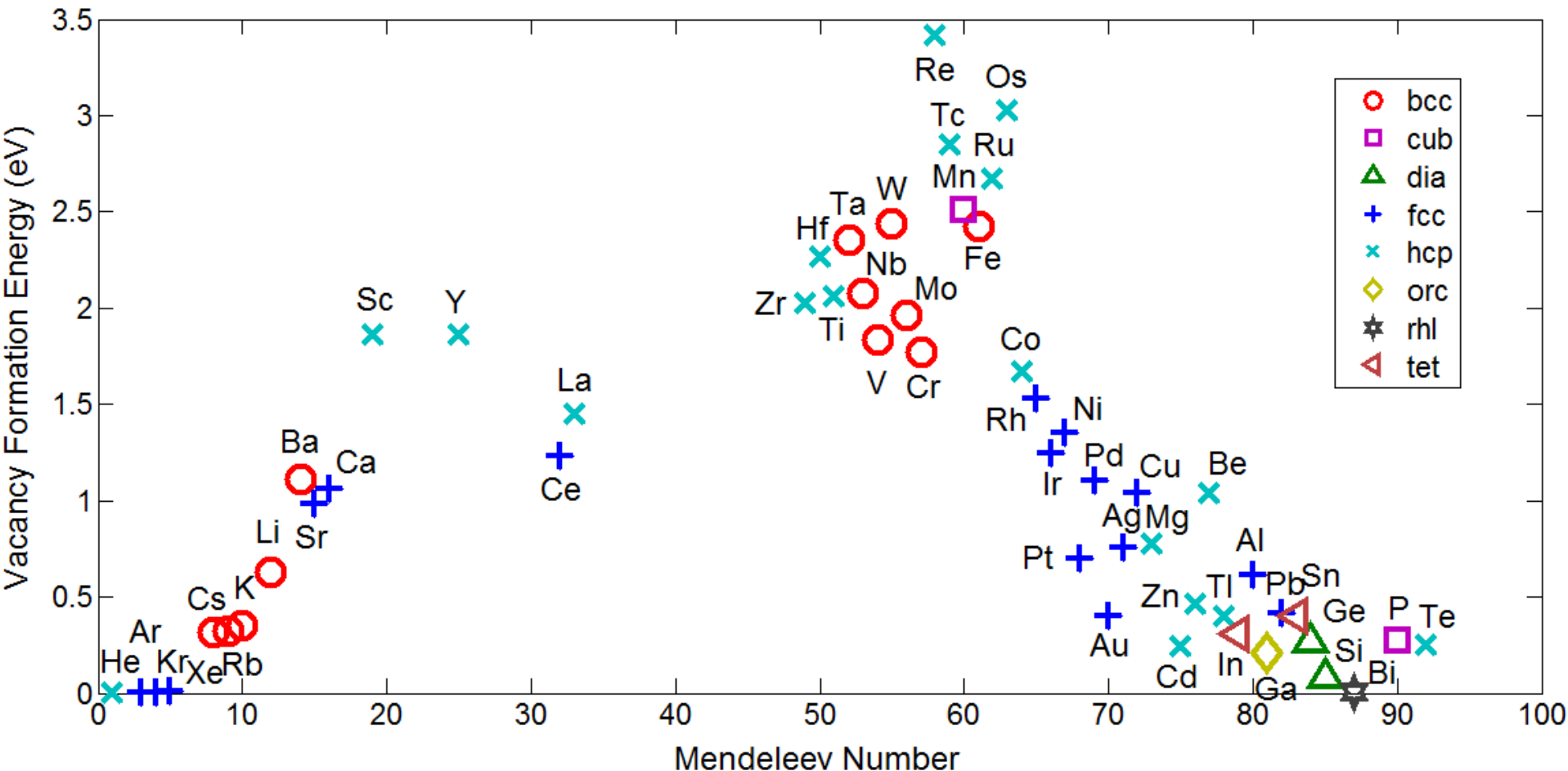
Trends with Descriptors: FCC H_{vf} Vs. Mendeleev Number



Trends with Descriptors: FCC H_{mig} Vs. Mendeleev Number

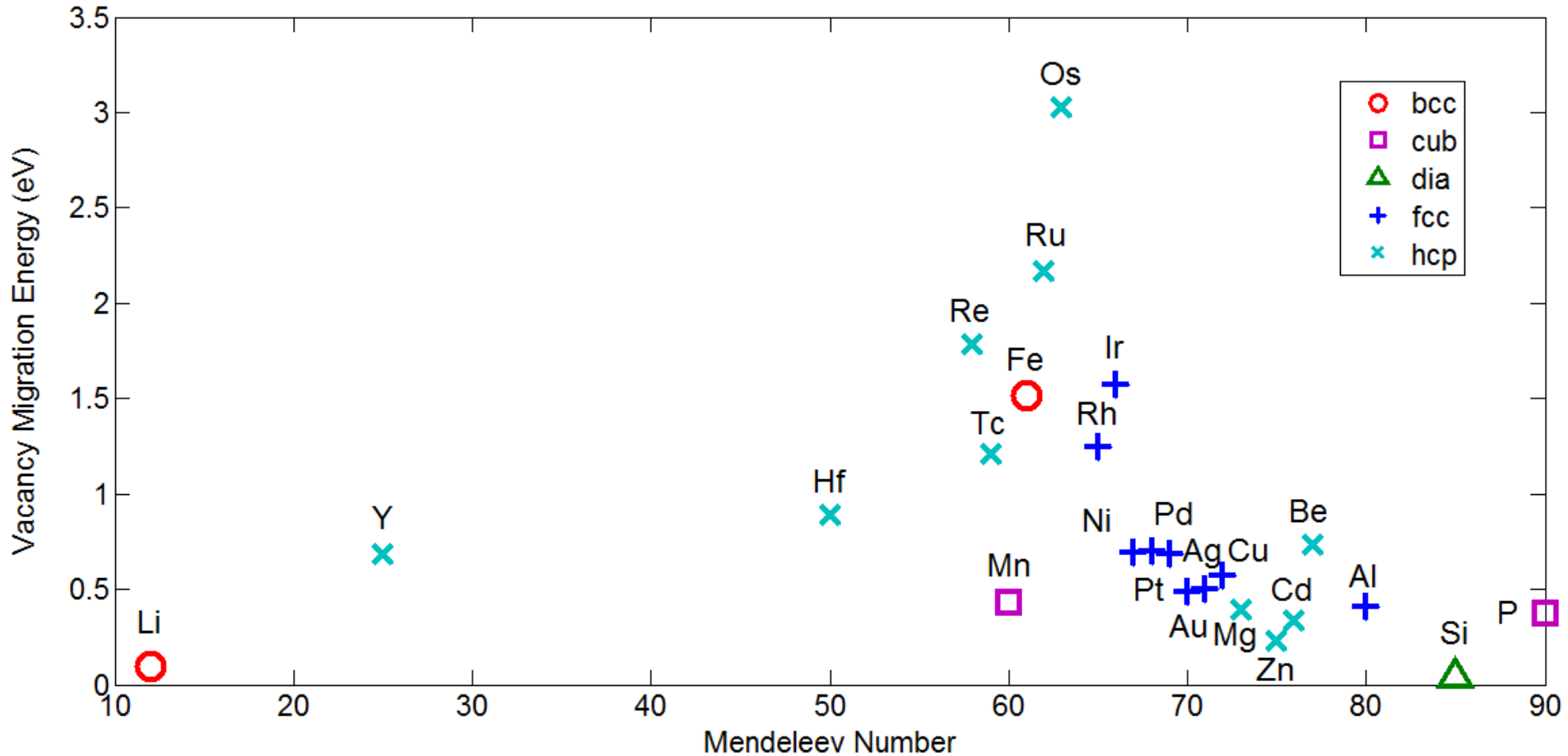


Trends with Descriptors: HCP H_{vf} Vs. Mendeleev Number

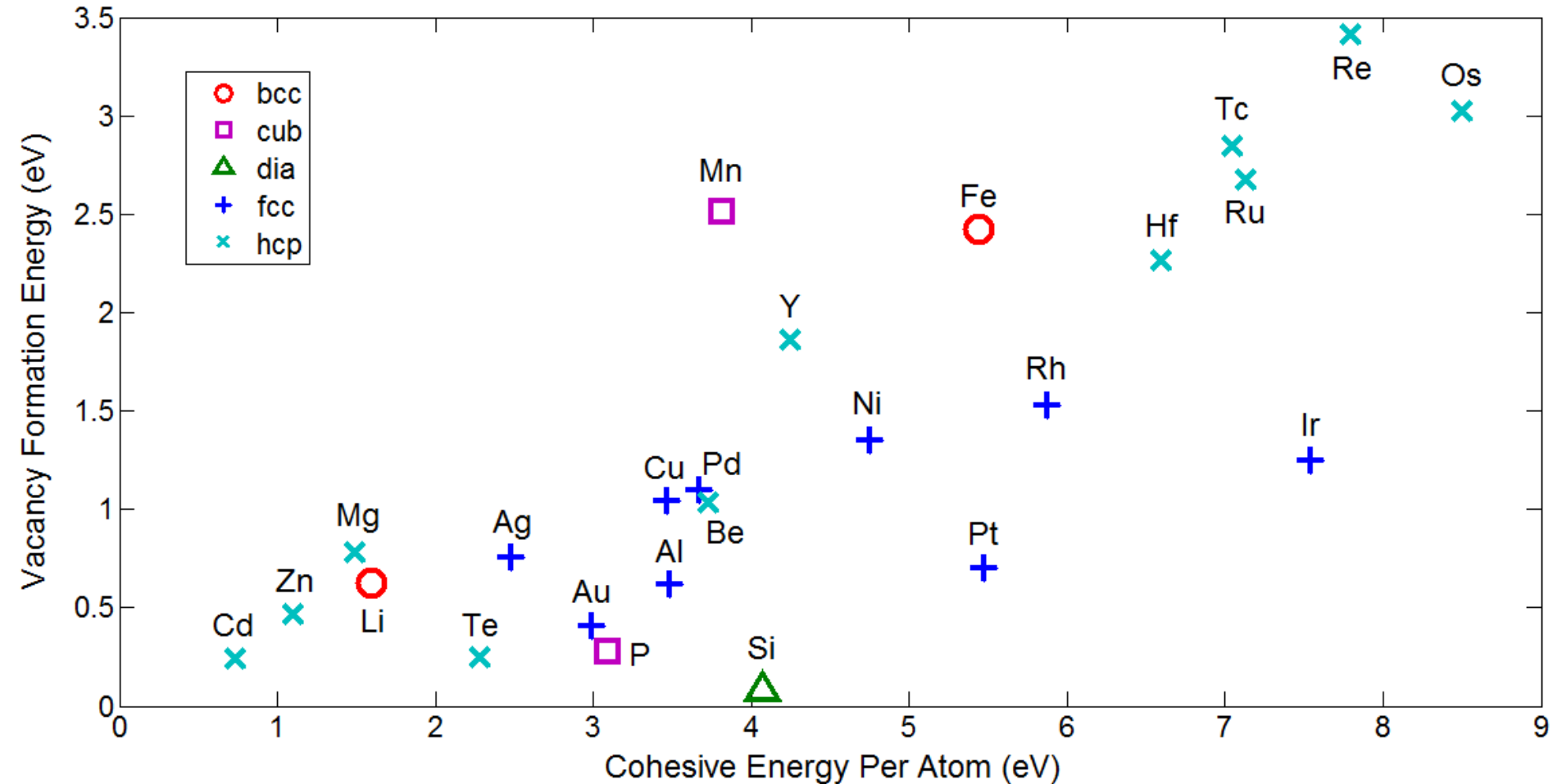


Trends with Descriptors: HCP Basil

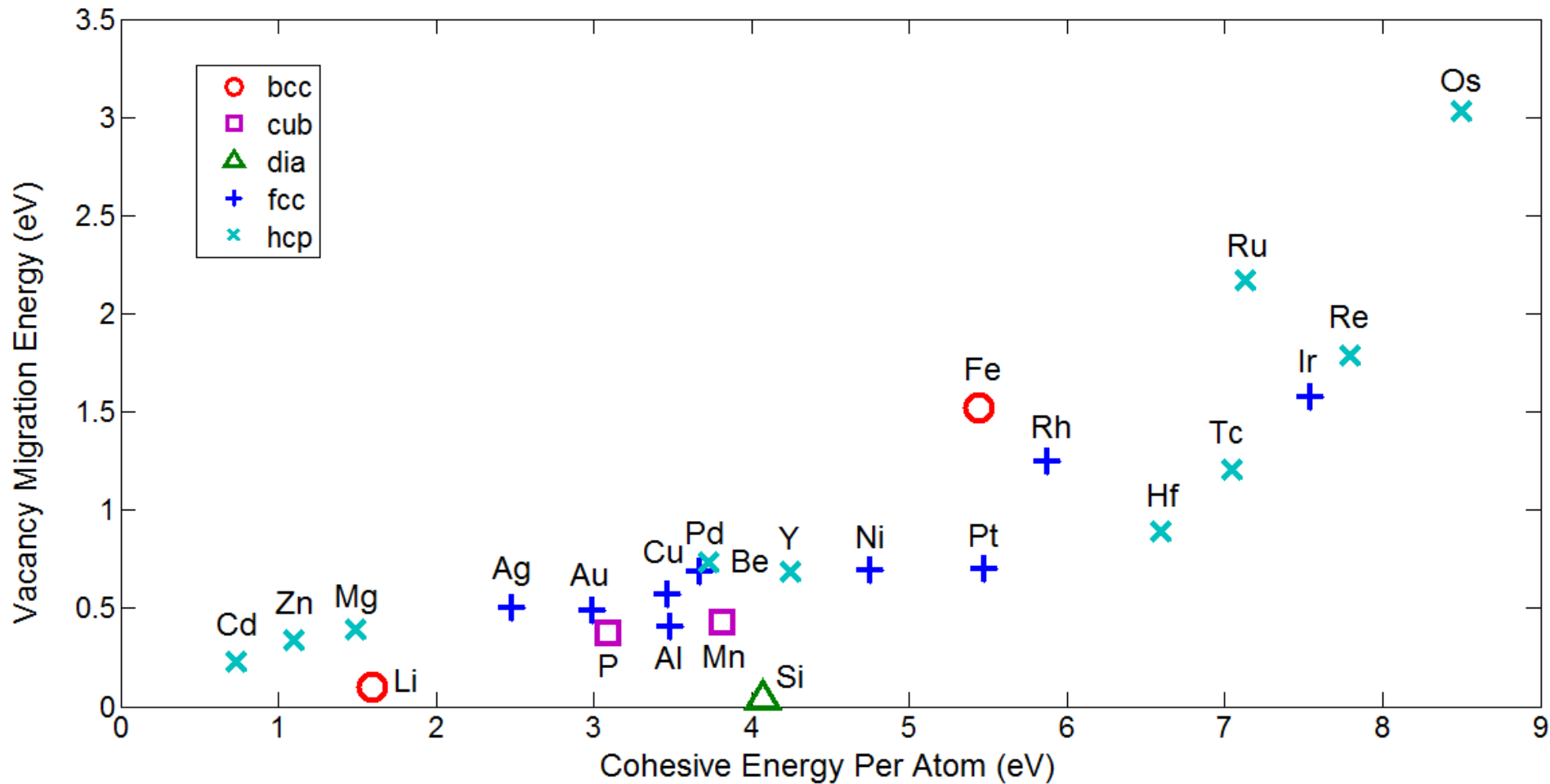
H_{mig} Vs. Mendeleev Number



HCP Evac versus Ecoh/atom

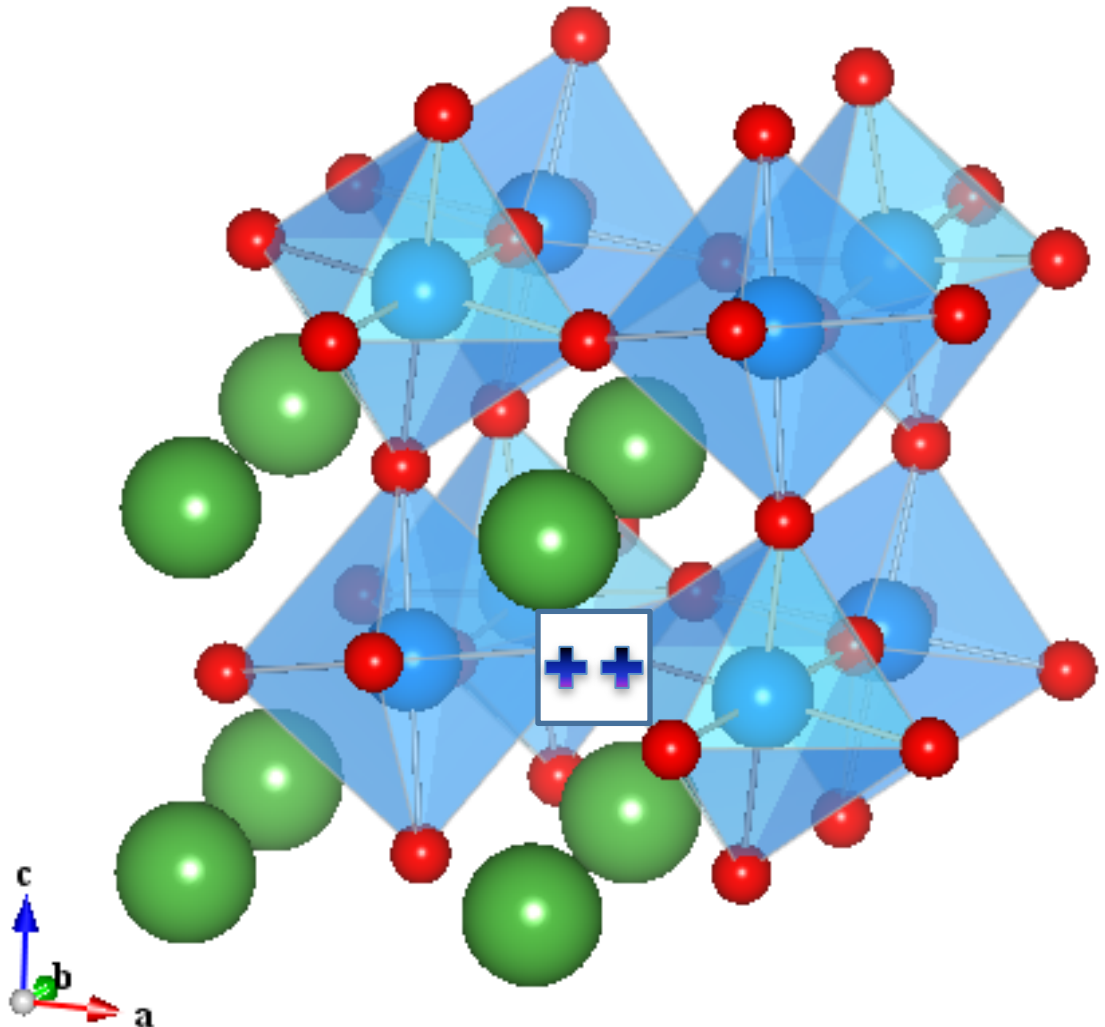


HCP Emig versus Ecoh/atom



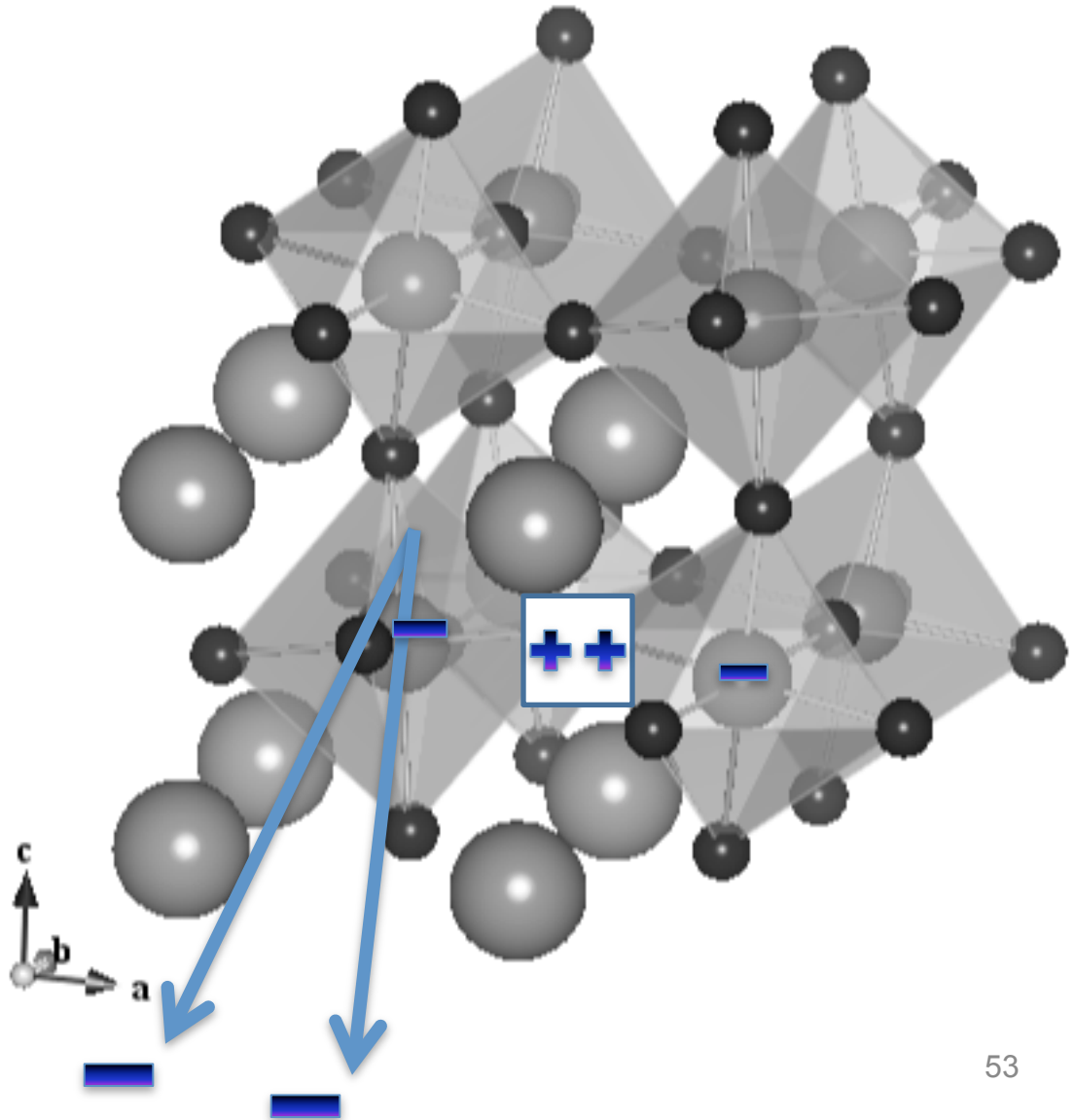
Modeling the vacancy

- The crystal expects an O^{2-} at the vacancy site,
- so the vacancy is a 'positive' defect with a +2 charge.
- For charge neutrality, the creation of each vacancy requires the handling of two extra electrons, or two 'negative' defects.

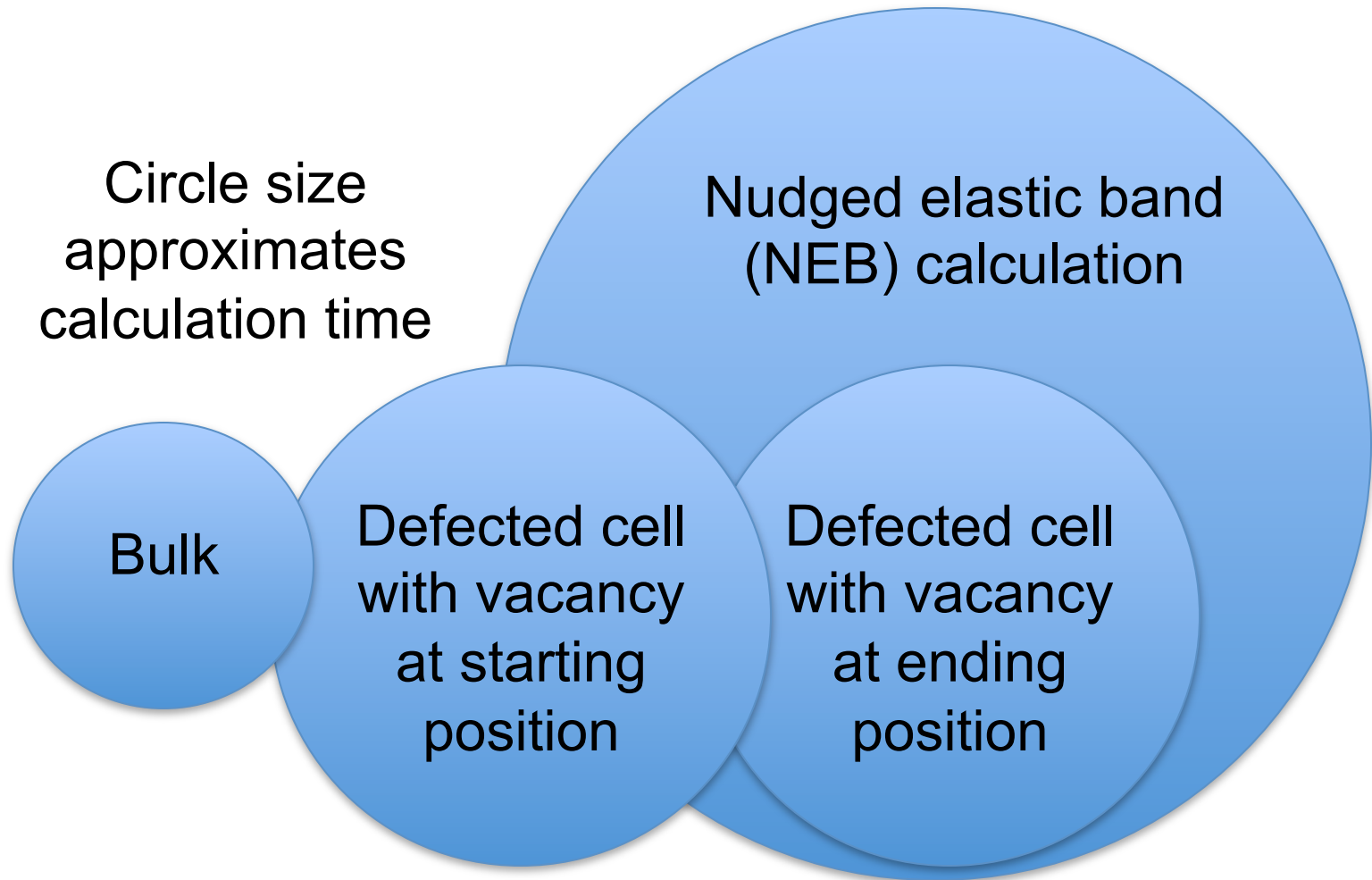


Modeling the vacancy

- We model the ‘negative’ defects by:
- 1) Removing two electrons to simulate defects outside the supercell:
“compensated”
- 2) Letting the supercell produce negative defects:
“uncompensated”



Can we screen for low barriers before doing a complete barrier calculation?



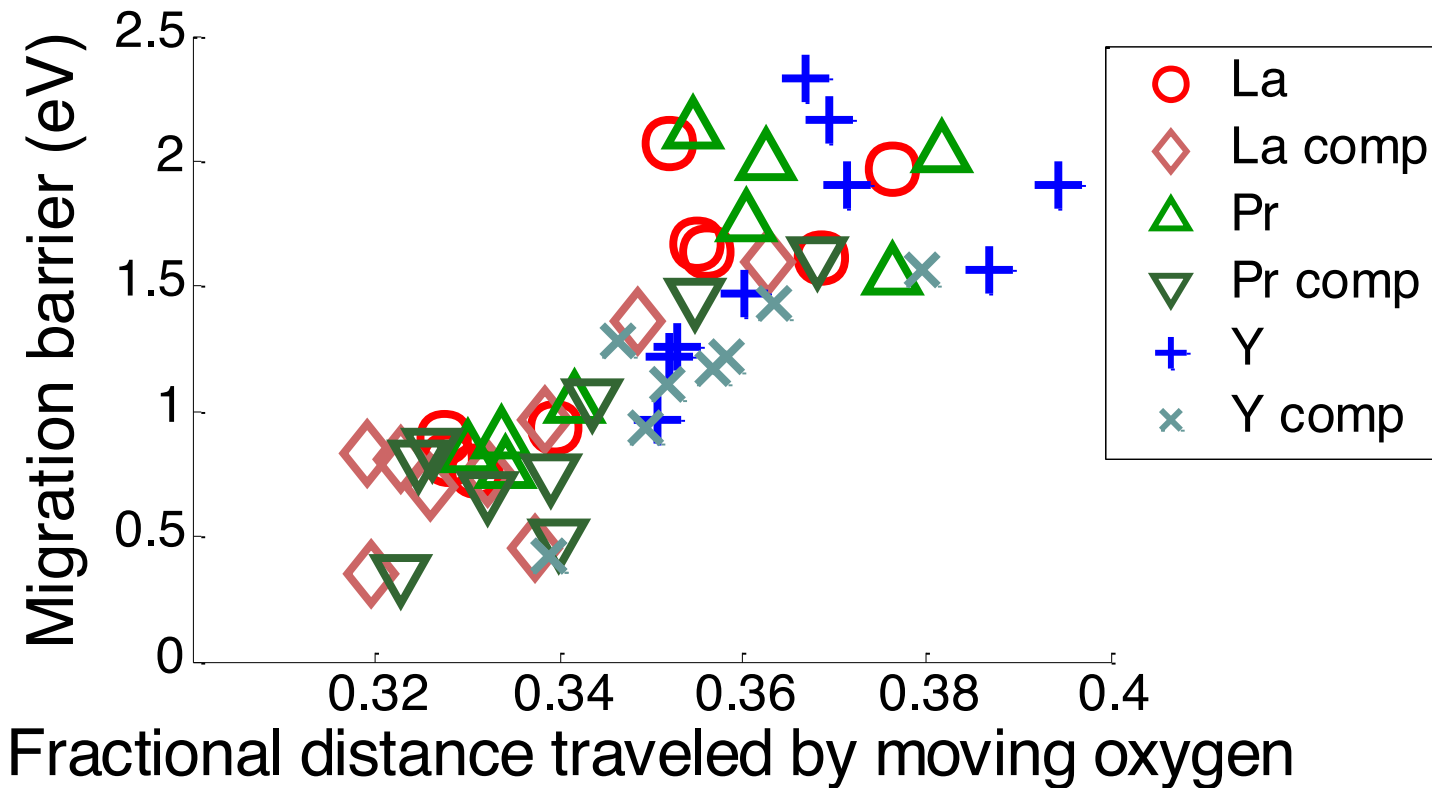
Descriptors That Did Not Correlate with Barrier

- Goldschmidt tolerance factor (cubic quality of unit cell, ability to form perovskite) and bulk cubic quality measures
- Kilner critical radius (defines triangle for oxygen to ‘squeeze’ through)
- B-site cation radius or electronegativity...
- But, some integrated effect of these and other factors may contribute to what we did find...

Sammells et al., Solid State Ionics **52**, 111-123 (1992).

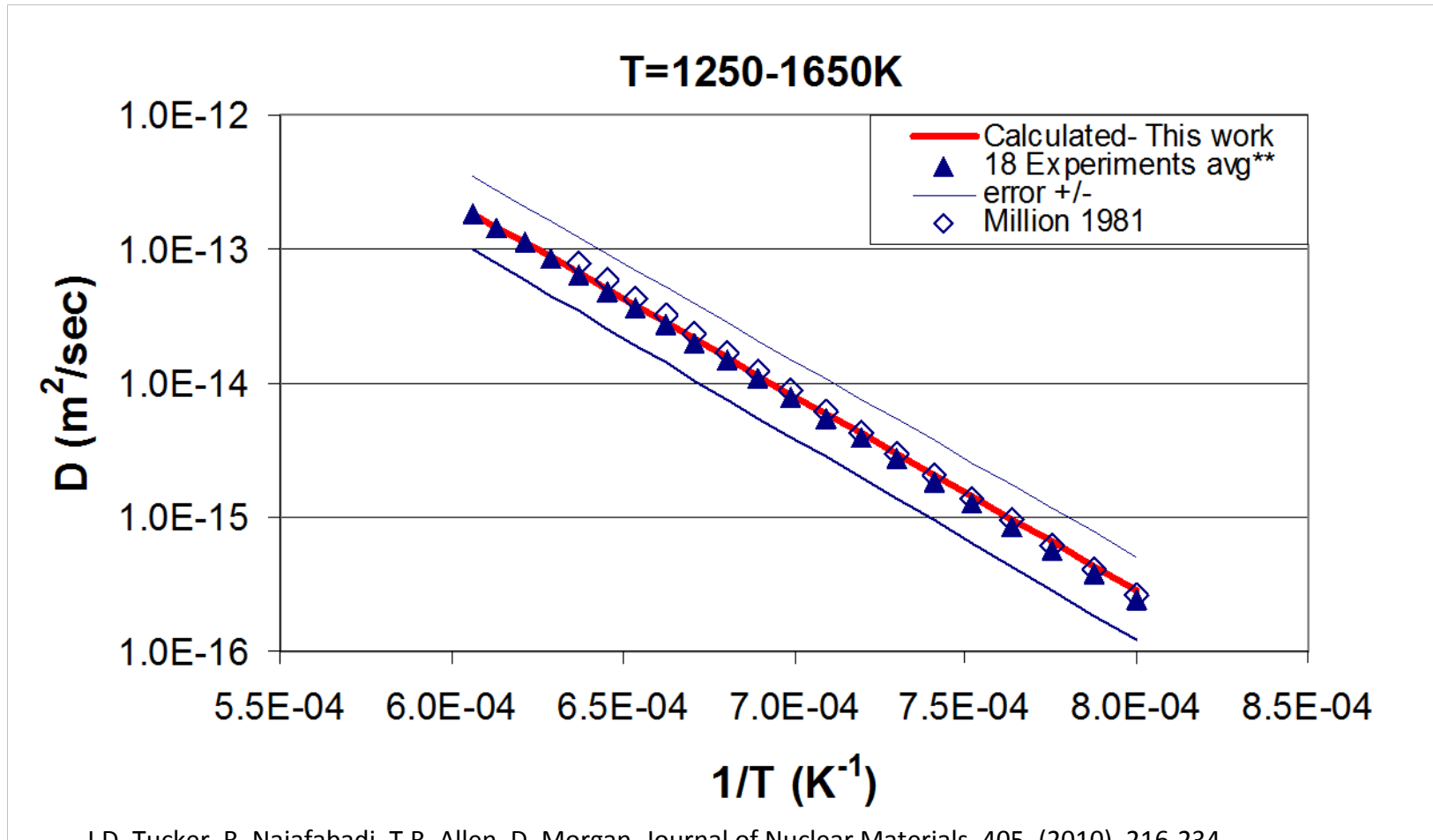
Mogensen et al., Solid State Ionics **174**, 279-286 (2004).

Shorter Travel Distance Correlates with Lower Barriers

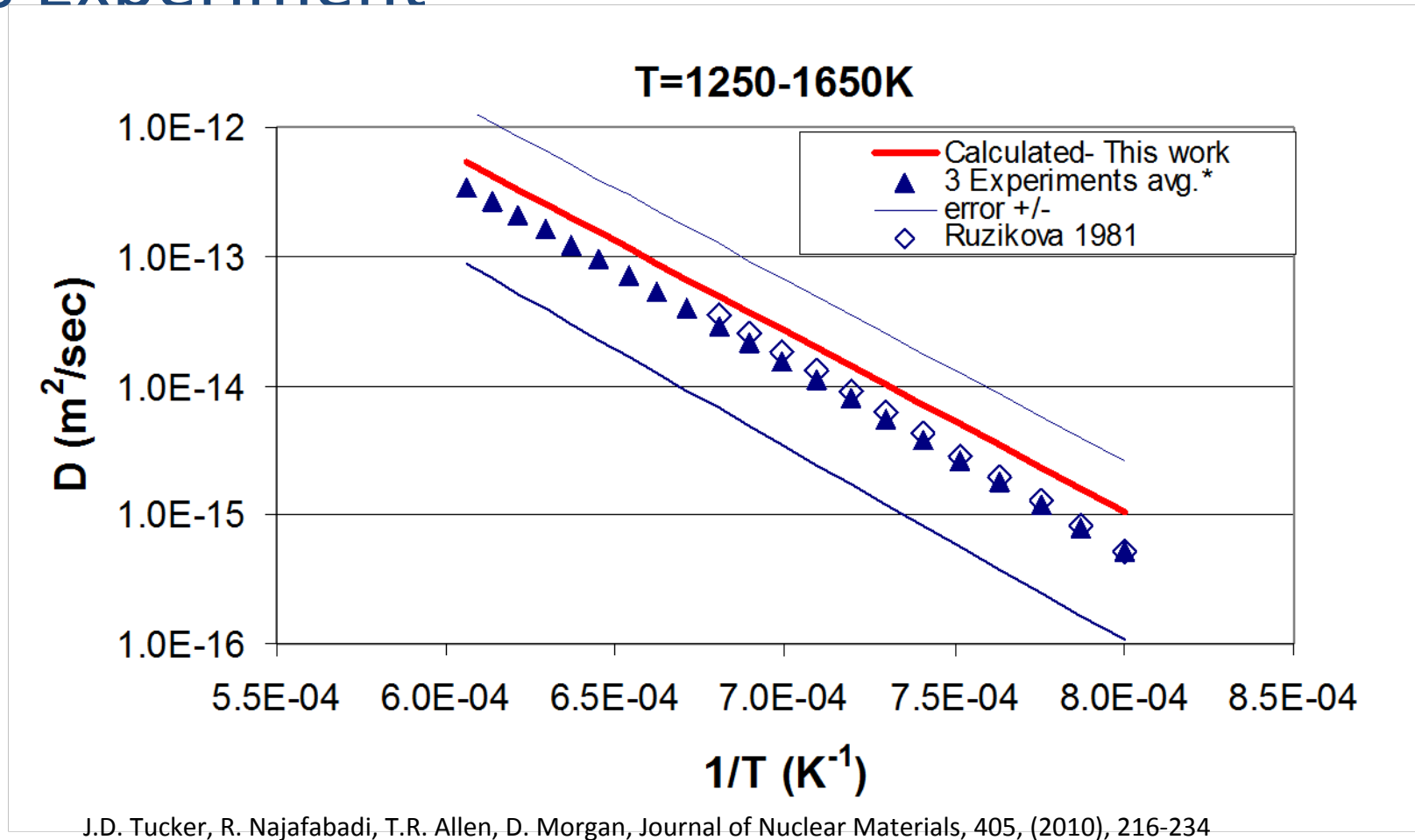


- Shows that structural geometry is playing a key role.
- But path length is no easier to get than Emig, so need a descriptor easier to calculate.

Ni Vacancy Self Diffusion – *Ab initio* vs Experiment

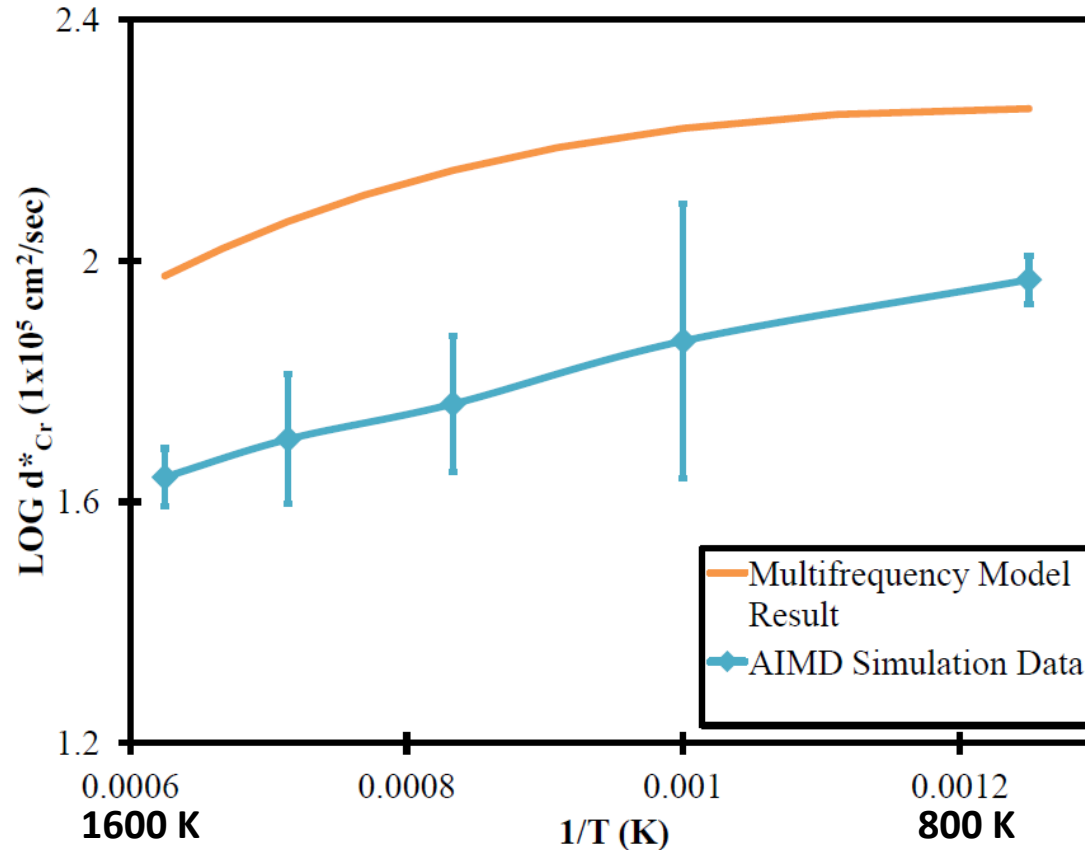


Cr Vacancy Impurity Diffusion in Ni – *Ab initio* vs Experiment



- For Ni self diffusion and Cr impurity diffusion, the *ab initio* values agree well with experiment.

Dilute Cr Interstitial Diffusion in Ni: Multifrequency vs AIMD



- Excellent agreement – discrepancy due to attempt frequency being approximated in multifrequency model
- The unusual T dependence of D_{Cr} in the dilute limit is reproduced.