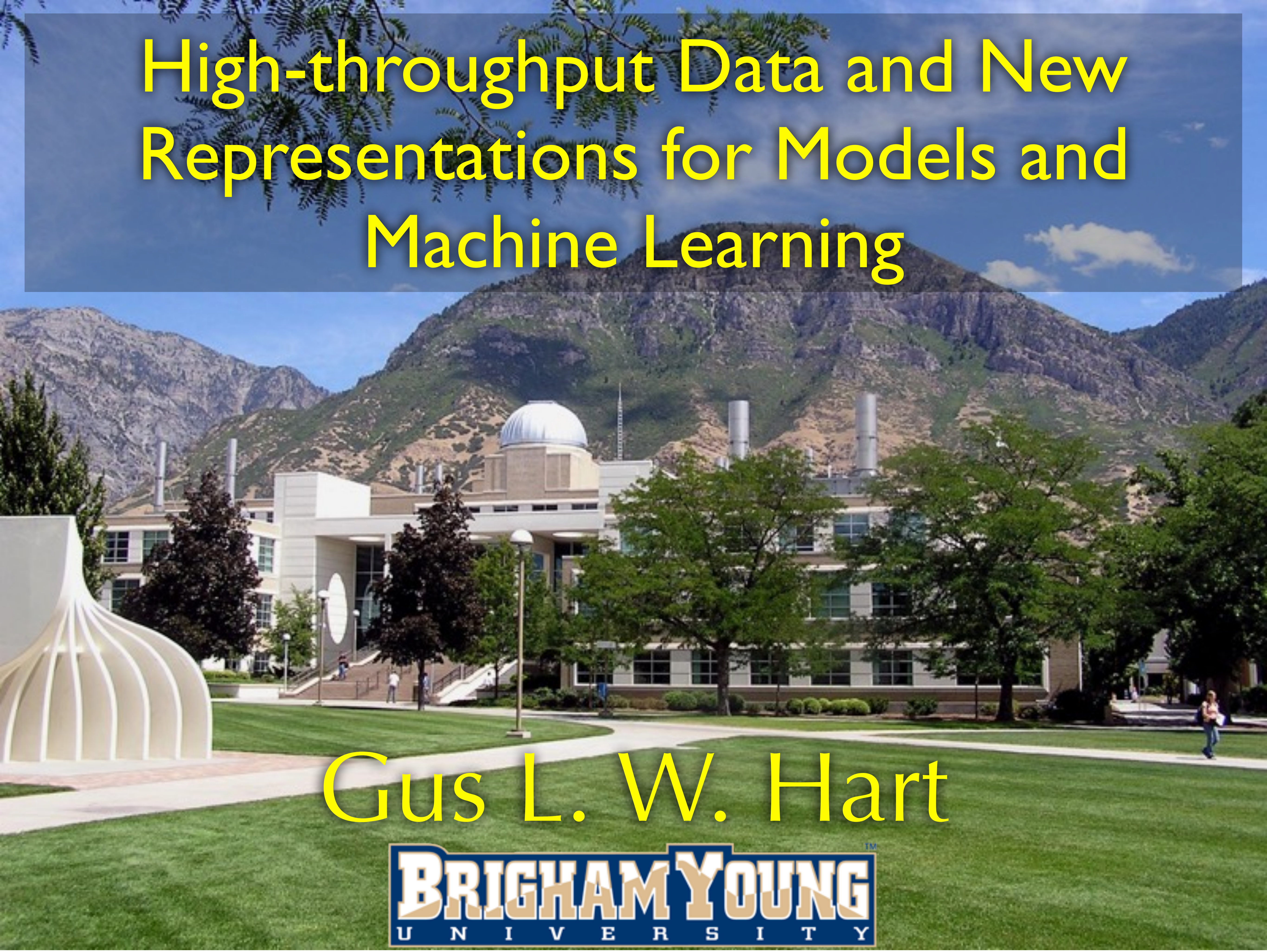
High-throughput Data and New Representations for Models and Machine Learning

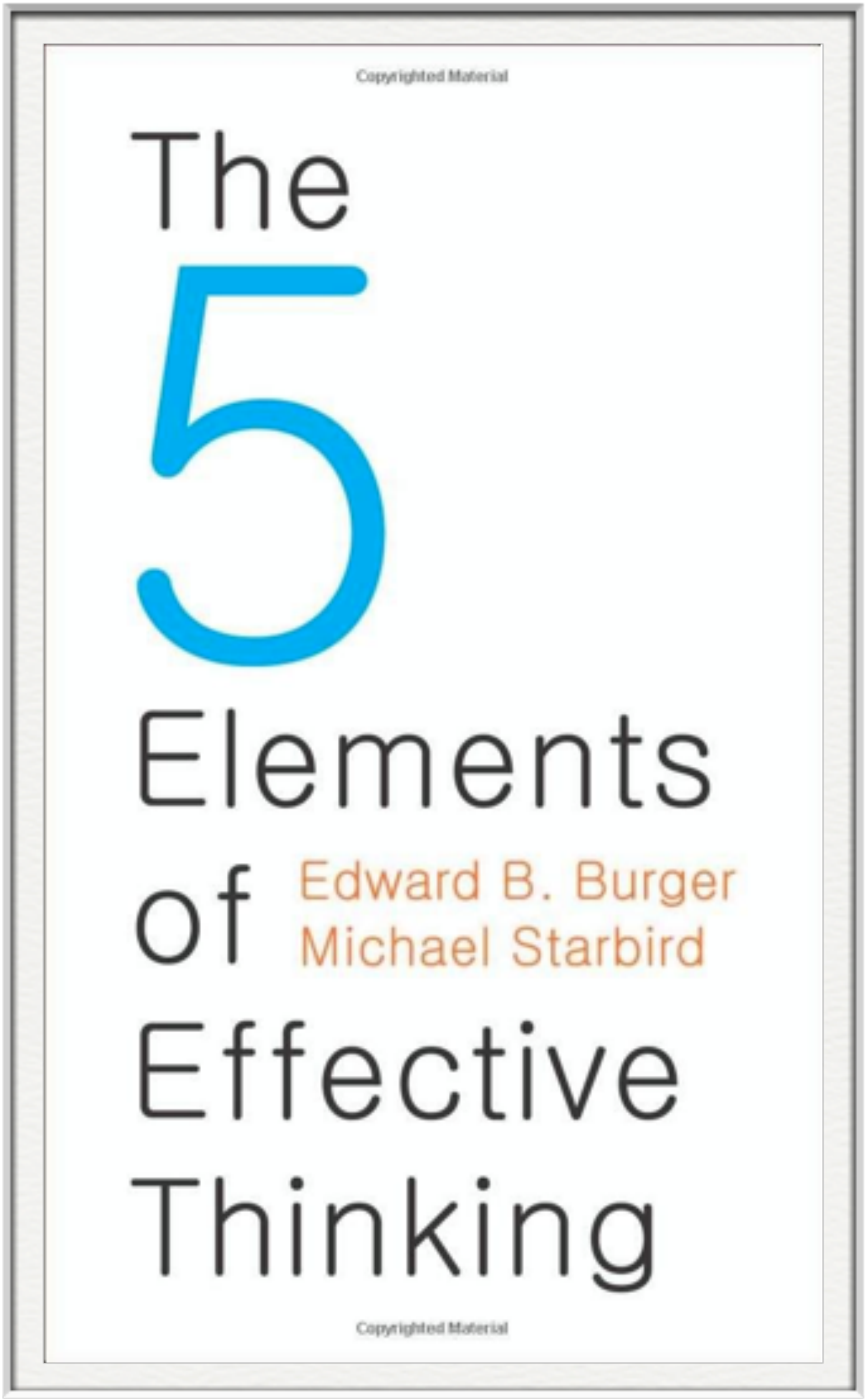


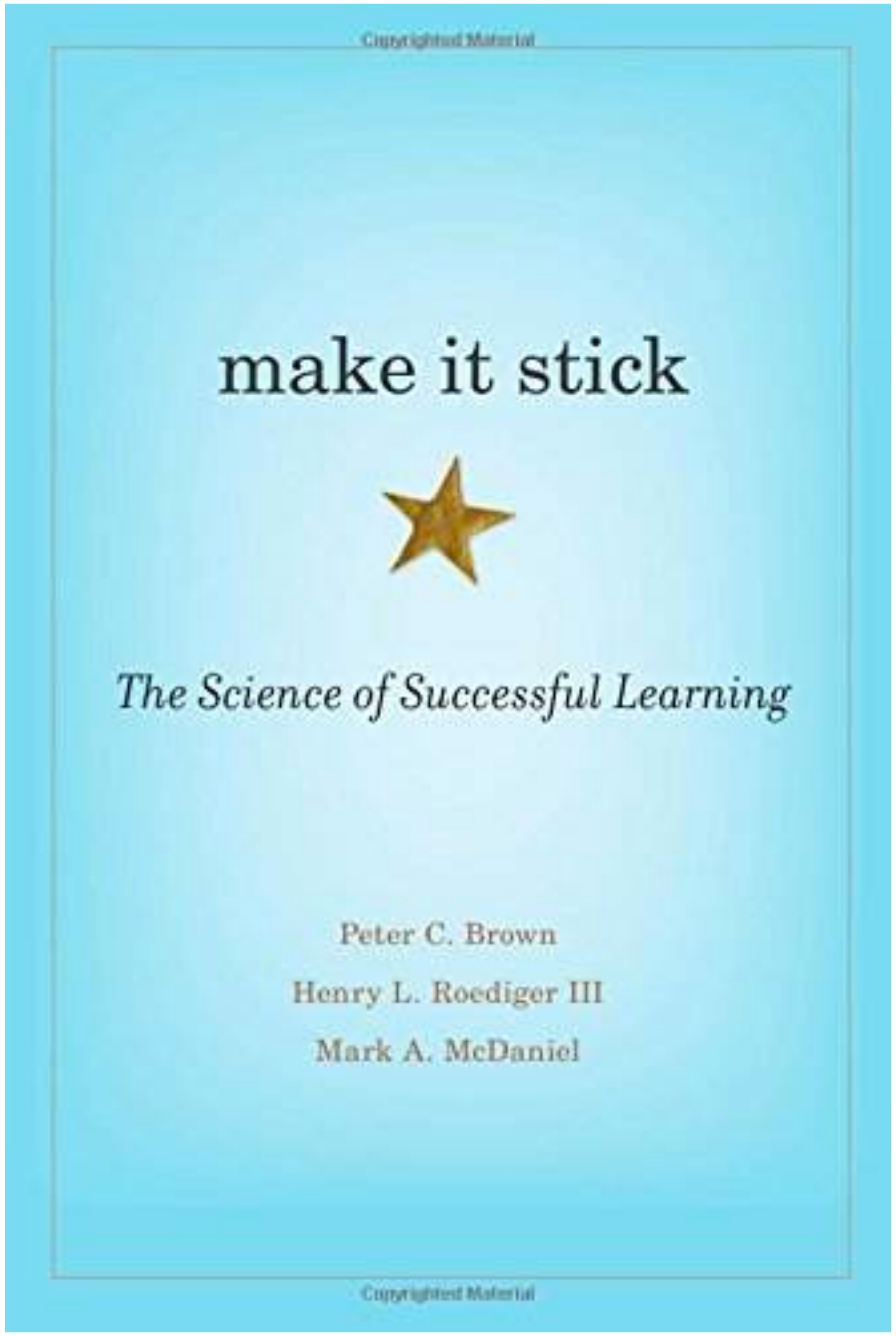
Gus L. W. Hart

Brigham Young University

Why am I here?

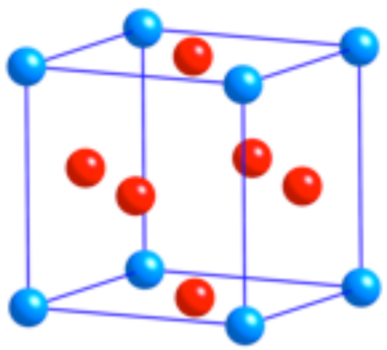
This talk is for you, not for me





High-Throughput Alloy Search

Experimental Structures (ICSD)



High-Throughput Alloy Search

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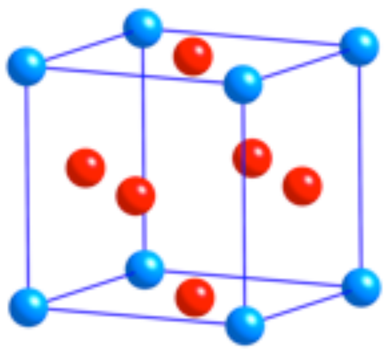

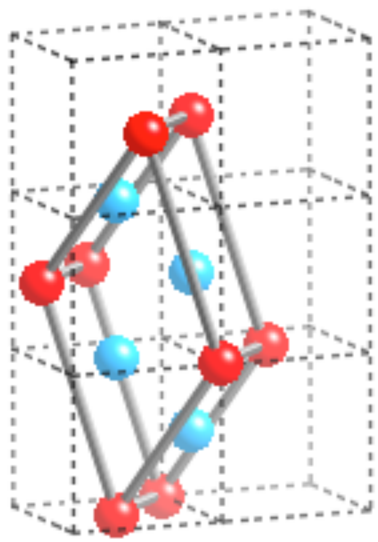

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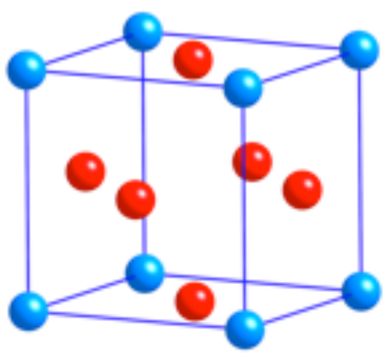

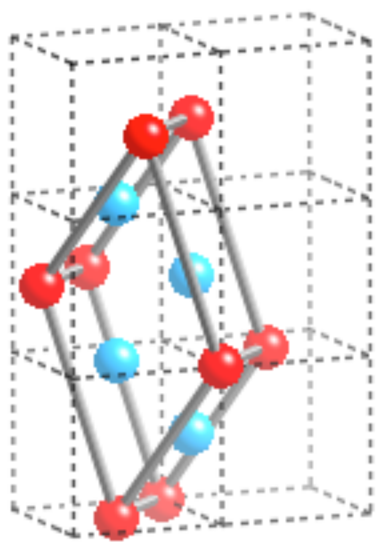

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High-Throughput Alloy Search

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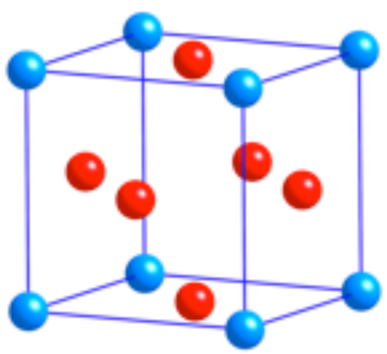

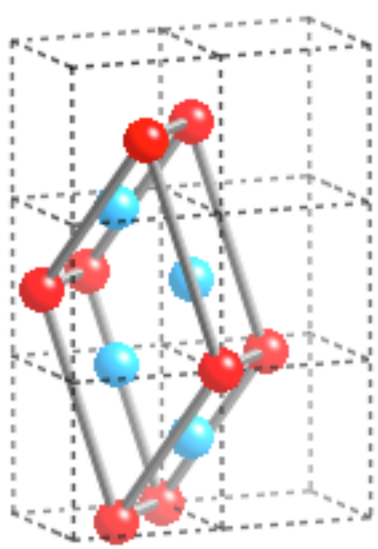

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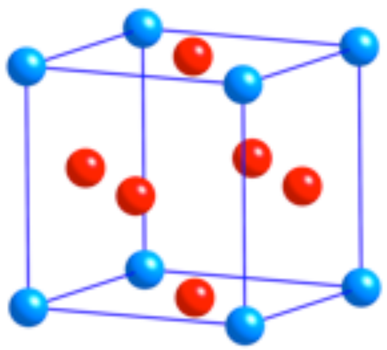
Combinatorial Substitution

High-Throughput Alloy Search

Experimental Structures (ICSD)



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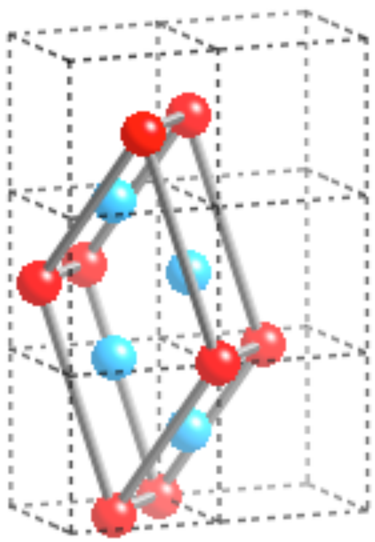

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Combinatorial Substitution

High-Throughput Alloy Search

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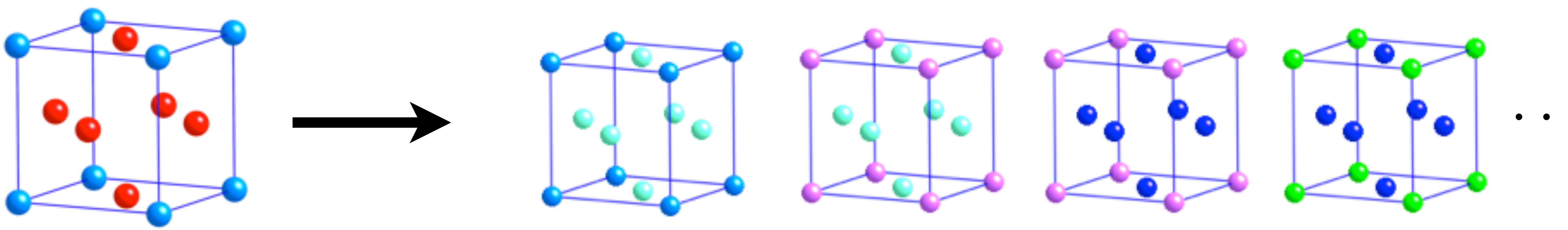
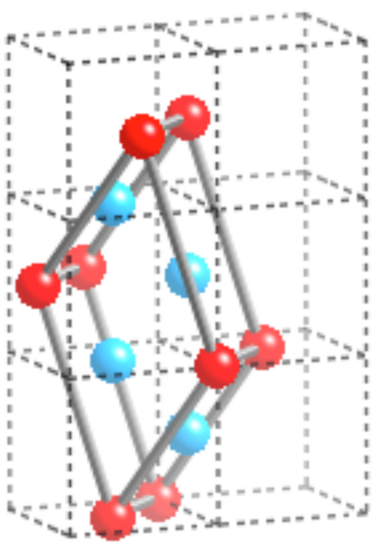
Combinatorial Substitution





High-Throughput Alloy Search

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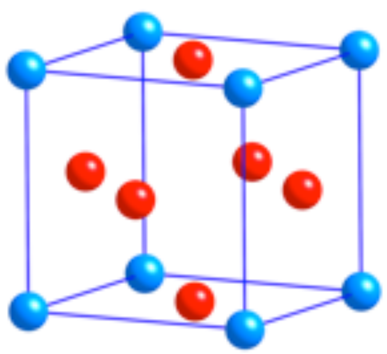
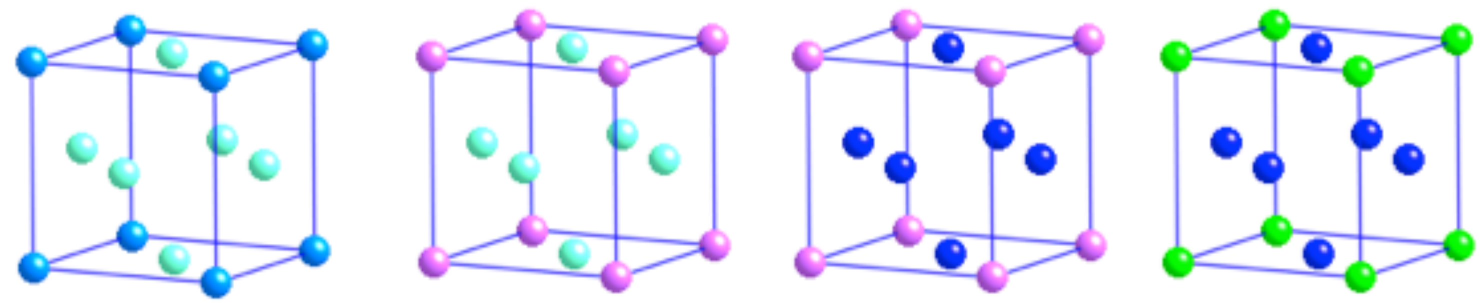
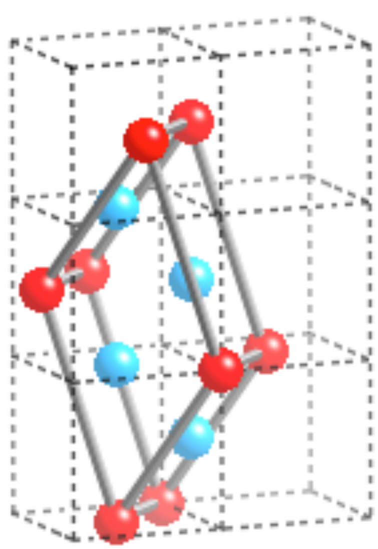
Combinatorial Substitution







High-Throughput Alloy Search

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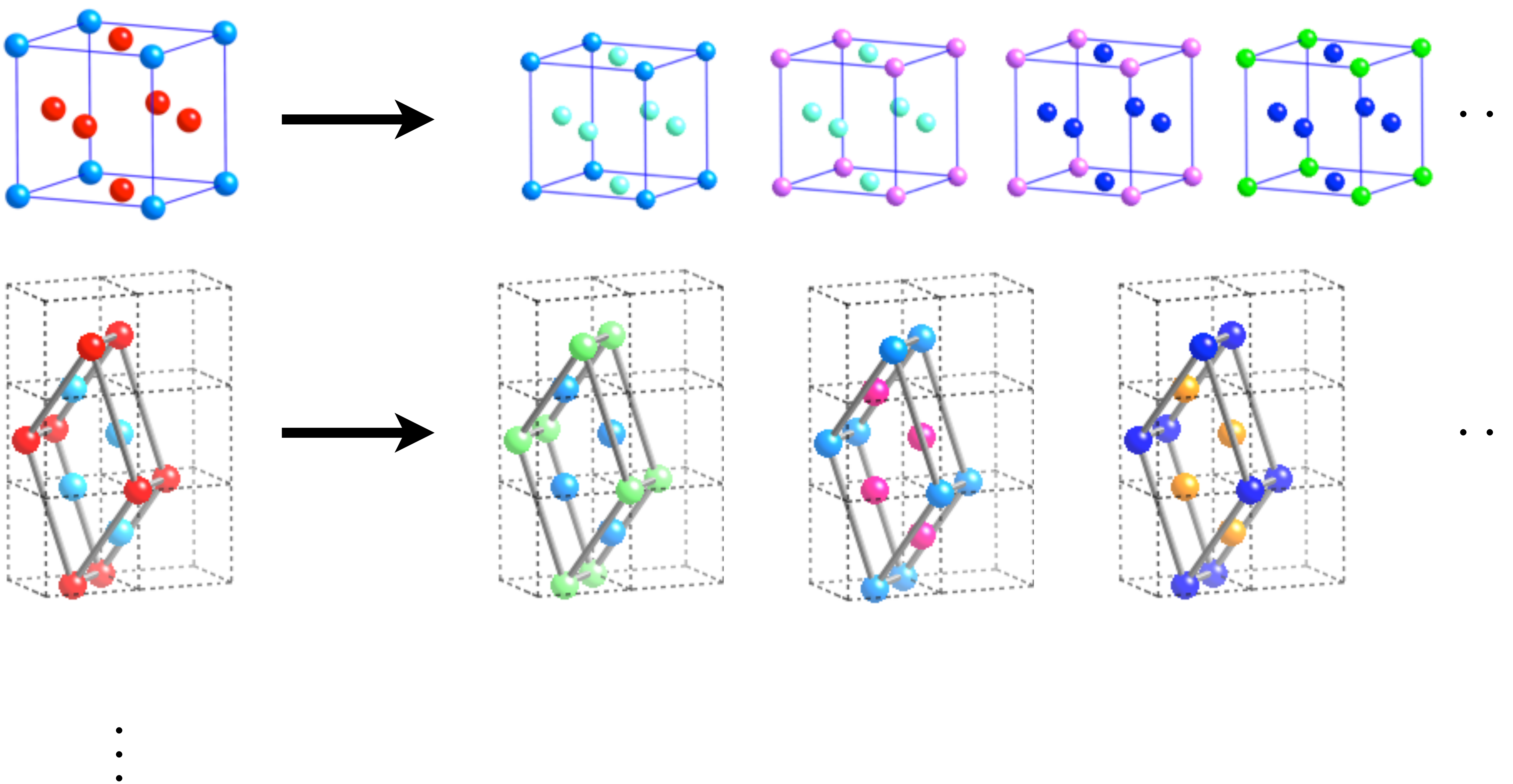
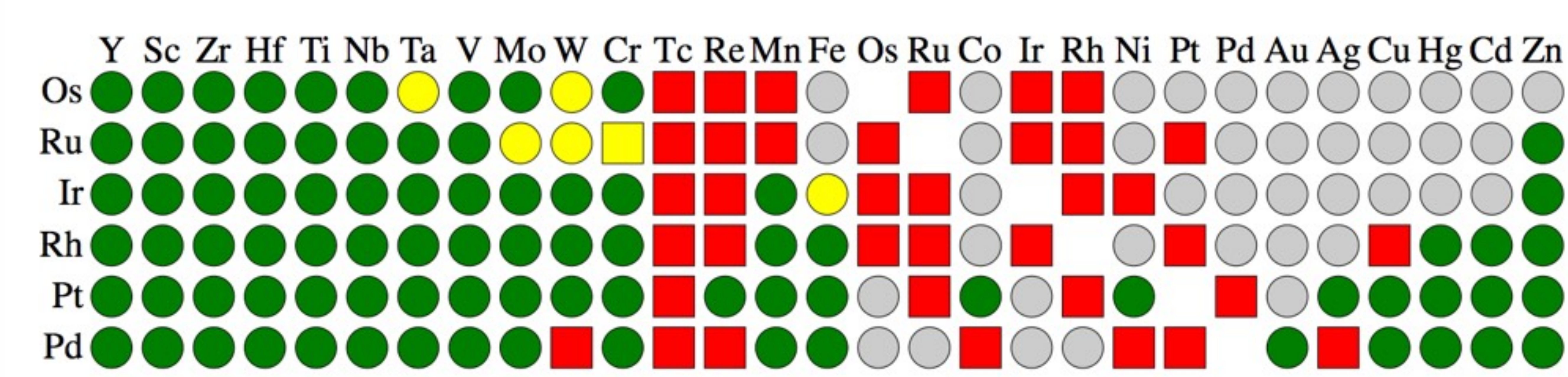


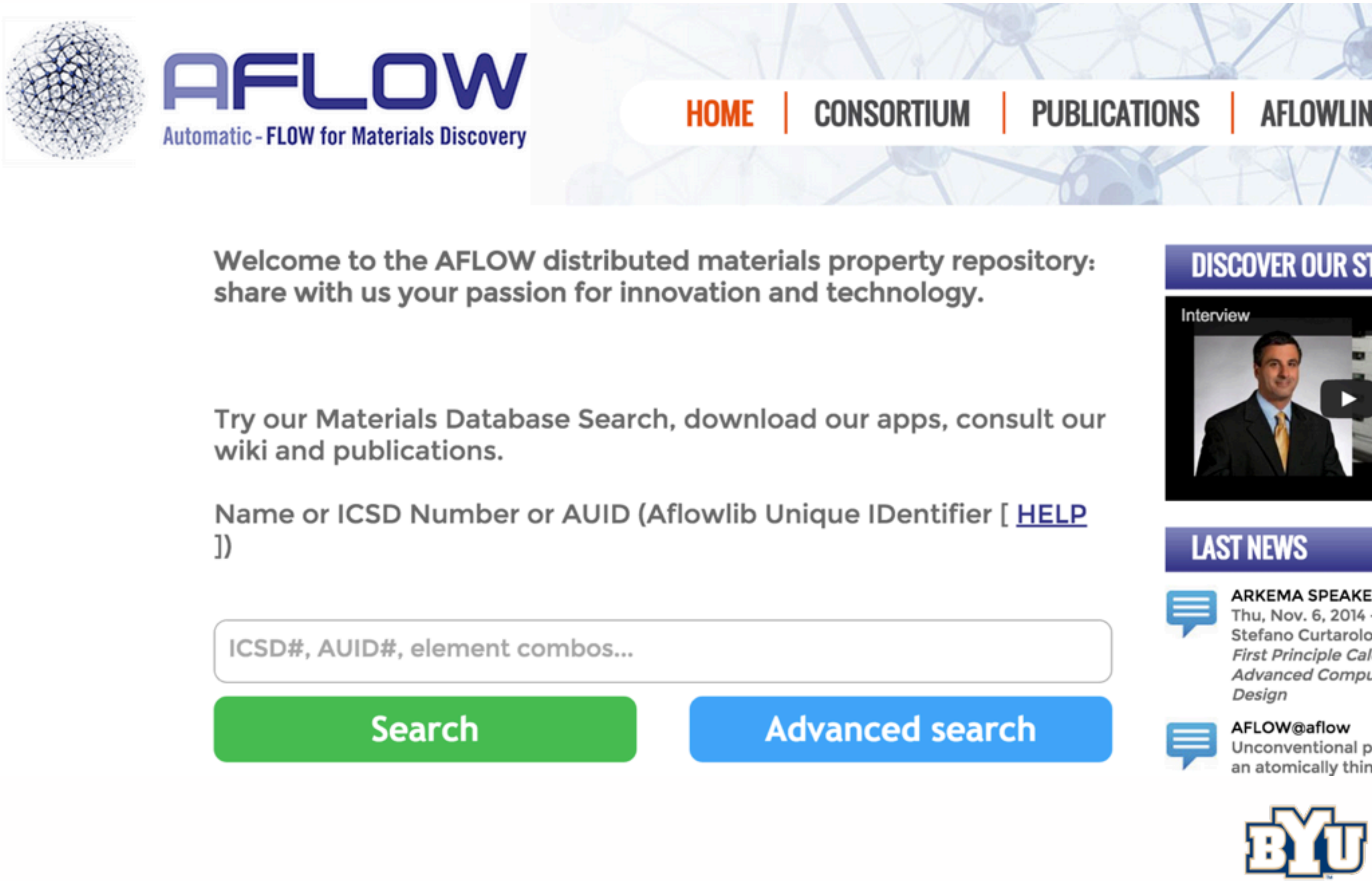
An Application: 153 Platinum-Group Alloys



Gus L.W. Hart, Stefano Curtarolo, Thaddeus B. Massalski, Ohad Levy;
Phys. Rev. X, **3** 041035 (Dec. 30 2013). (msg.byu.edu/pubs.php)

Viewpoint: Computational Materials Discovery Goes Platinum

http://aflowlib.org



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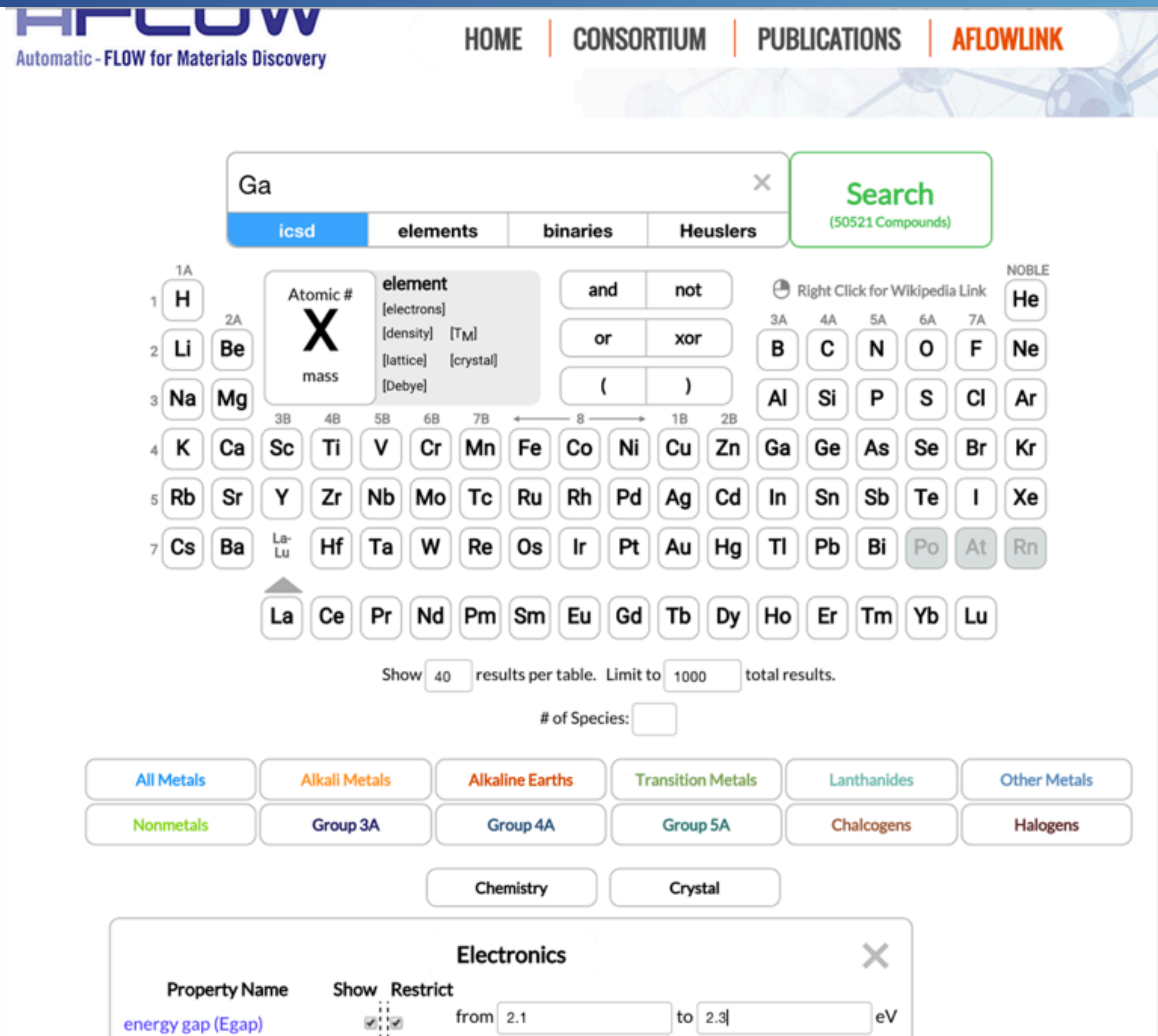


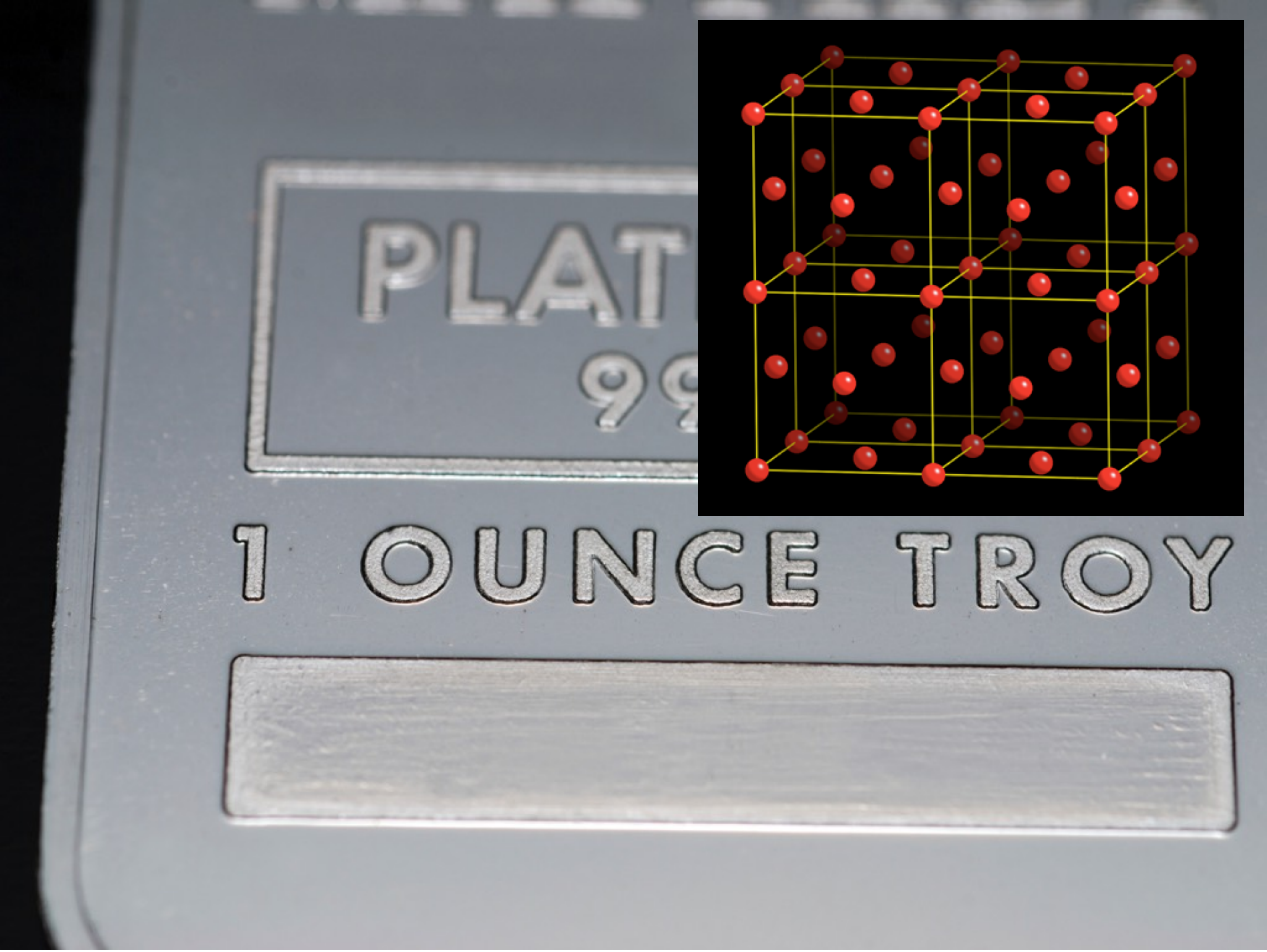
http://aflowlib.org

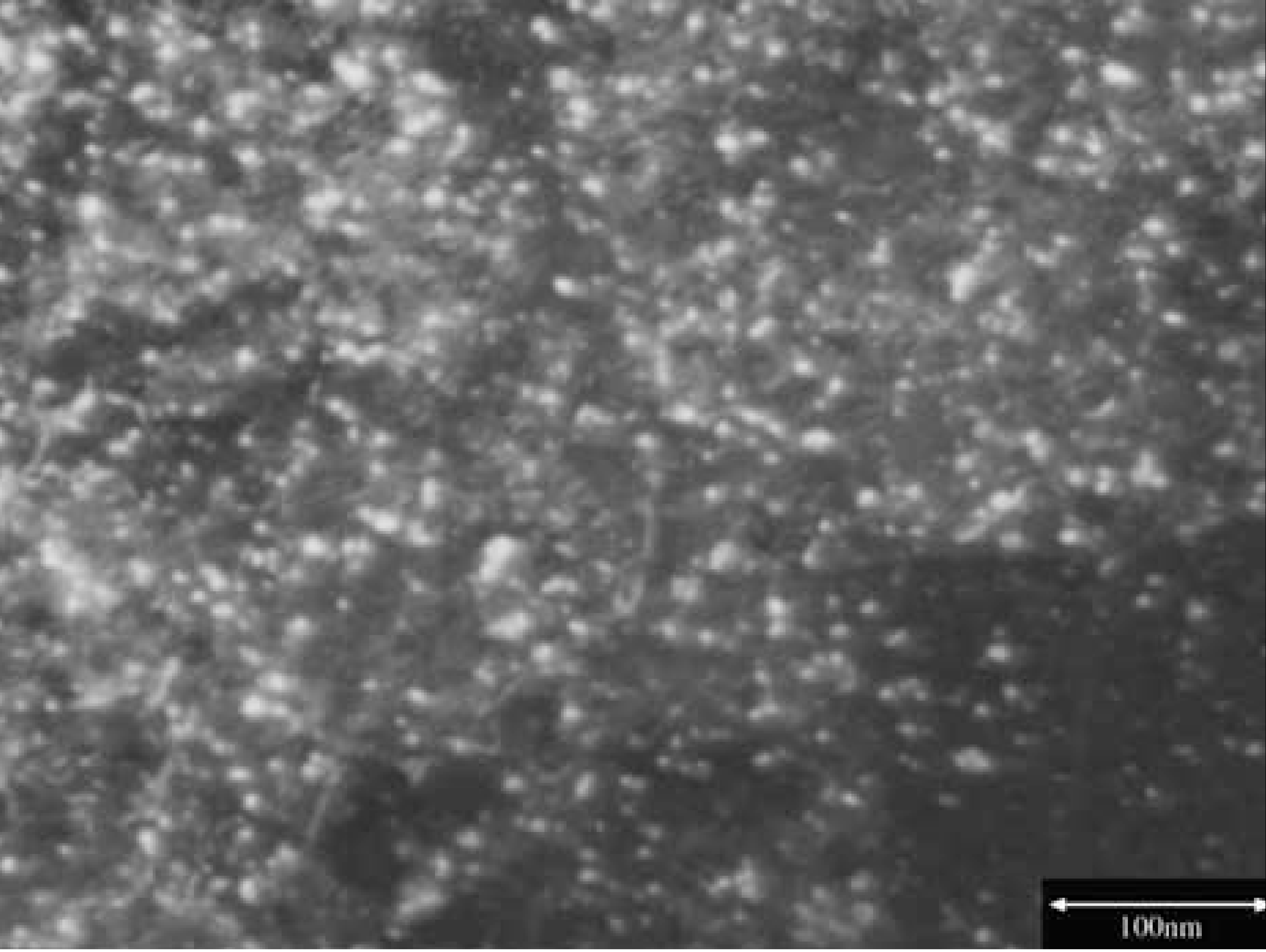
12	$Cd_1Ga_2S_4$	2.2029	e7585605e0bab007	ICSD_WEB/BCT/Cd1Ga2S4_ICSD_31354
13	$Cd_1Ga_2S_4$	2.2107	e904ea4649d40ae1	ICSD_WEB/BCT/Cd1Ga2S4_ICSD_25642
14	$Cl_4Ga_4Te_4$	2.2836	97bbe8d3a150a566	ICSD_WEB/ORC/Cl1Ga1Te1_ICSD_15582
15	$Cs_{12}Ga_4Se_{12}$	2.1331	e69e0608e64542e8	ICSD_WEB/MCL/Cs6Ga2Se6_ICSD_35293
16	$Er_6Ga_2S_{12}$	2.1403	08731daf3a7f012d	ICSD_WEB/ORCC/Er3Ga1S6_ICSD_2511
17	$Ga_2Ge_4O_{14}Pb_3$	2.2086	a990ebca004332af	ICSD_WEB/HEX/Ga2Ge4O14Pb3_ICSD_250123
18	$Ga_2Mn_1S_4$	2.2604	8df034a523f2099f	ICSD_WEB/BCT/Ga2Mn1S4_ICSD_152909
19	$Ga_2O_4Tl_2$	2.1148	bf2c2af810b2f5ec	ICSD_WEB/RHL/Ga1O2Tl1_ICSD_33579
20	$Ga_2S_4Zn_1$	2.1564	2015176ca138b0e3	ICSD_WEB/TET/Ga2S4Zn1_ICSD_635300
21	$Ga_4Ge_1O_8$	2.136	96eeb0c60e611111	ICSD_WEB/MCLC/Ga4Ge1O8_ICSD_202044
22	$Ga_4I_{12}Li_4$	2.2612	7e2dc466f1442b07	ICSD_WEB/MCL/Ga1I3Li1_ICSD_202642
23	$Ga_4Li_4Se_8$	2.1189	44e3dfa0e77246f9	ICSD_WEB/ORC/Ga1Li1Se2_ICSD_634546
24	$Ga_4Li_4Se_8$	2.1651	e5d89371a9e11bb0	ICSD_WEB/ORC/Ga1Li1Se2_ICSD_96915
25	Ga_4O_6	2.1608	245ca11a8709306f	ICSD_WEB/MCLC/Ga2O3_ICSD_603563
26	Ga_4O_6	2.1538	43a955013462937a	ICSD_WEB/MCLC/Ga2O3_ICSD_184327
27	Ga_4O_6	2.1734	c980db287f78262c	ICSD_WEB/MCLC/Ga2O3_ICSD_166198
28	Ga_4O_6	2.1656	cb24f97fe2c1198c	ICSD_WEB/MCLC/Ga2O3_ICSD_83645
29	Ga_4O_6	2.1702	e8dbaa09cef83775	ICSD_WEB/MCLC/Ga2O3_ICSD_34243
30	$Ga_4P_4S_{16}$	2.2855	d5209efc85921c33	ICSD_WEB/MCL/Ga1P1S4_ICSD_2613
31	$Ga_6In_6S_{18}$	2.145	c2c67ddb664c3a14	ICSD_WEB/HEX/Ga1In1S3_ICSD_62929
32	Ga_8I_{12}	2.2109	9758f7460f79ec5a	ICSD_WEB/MCL/Ga2I3_ICSD_24822
33	$Ga_9O_2S_{13}Tl_3$	2.2428	5593f5376b6d222c	ICSD_WEB/HEX/Ga9O2S13Tl3_ICSD_61256

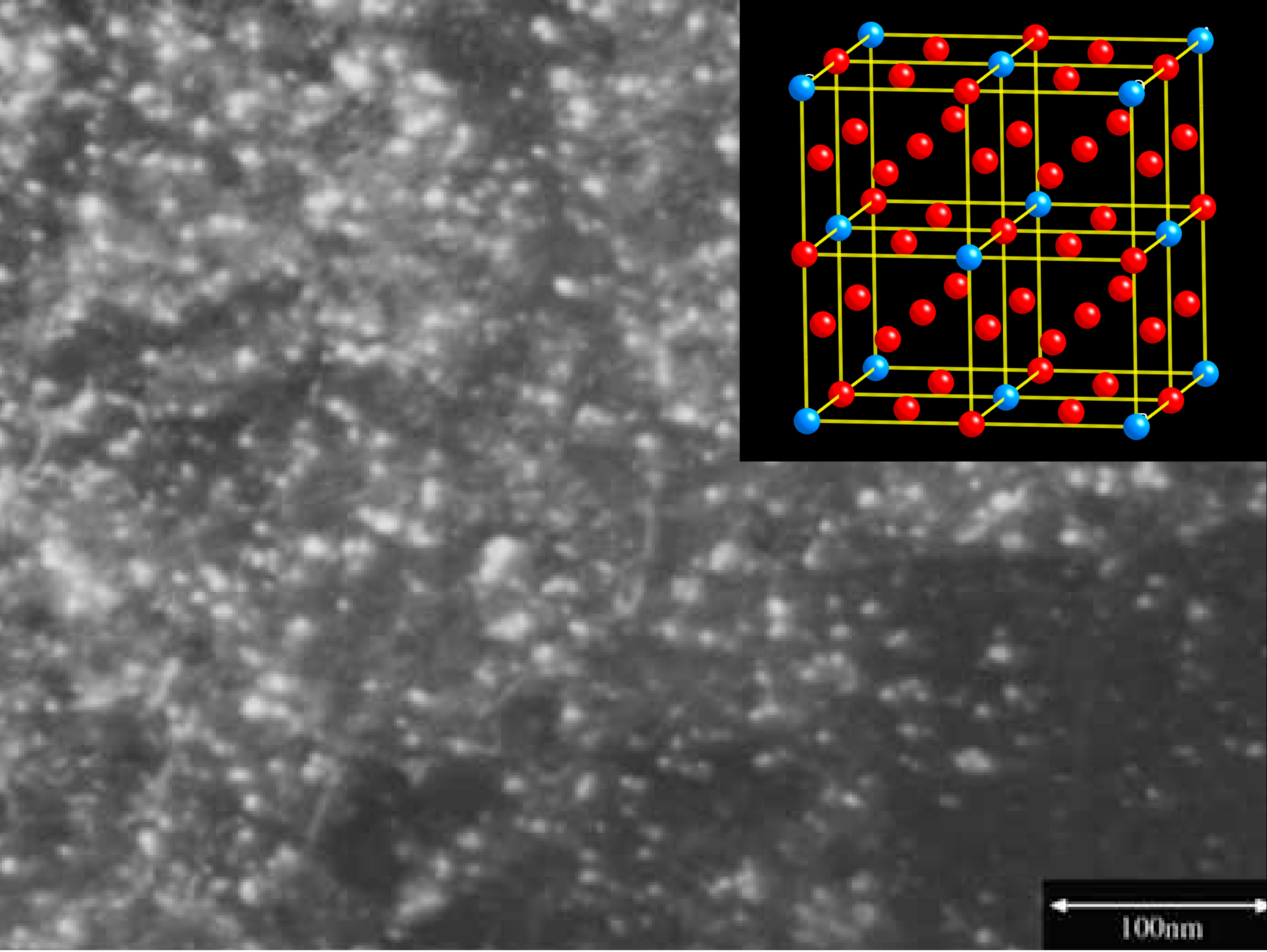
[1] R. H. Taylor, F. Rose, C. Toher, O. Levy, M. Buongiorno Nardelli, and S. Curtarolo, *A RESTful API for exchanging Materials Data in the AFLOWLIB.org consortium*, Comp. Mat. Sci. VVV, PPP (2014). [doi] [pdf]
[2] W. Setyawan and S. Curtarolo, *High-throughput electronic structure calculations: challenges and tools*, Comp. Mat. Sci. **49**, 299-312 (2010) [doi] [pdf]
[3] W. Setyawan, R. M. Gaume, S. Lam, R. S. Feigelson, and S. Curtarolo, *High-Throughput Combinatorial Database of Electronic Band Structures for Inorganic Scintillator Materials*, ACS Comb. Sci. **13(4)**, 382-390 (2011) [doi] [pdf] [suppl]
[4] S.Wang, Z. Wang, W. Setyawan, N. Mingo, S. Curtarolo, *Assessing the thermoelectric properties of sintered compounds with high-throughput ab-initio calculations*, Phys. Rev. X **1**, 021012 (2011) [doi] [pdf] [suppl]
[5] G. Kresse, and J. Hafner *Ab initio molecular dynamics for liquid metals*, Phys. Rev. B **47**, 558-561 (1993) [doi]

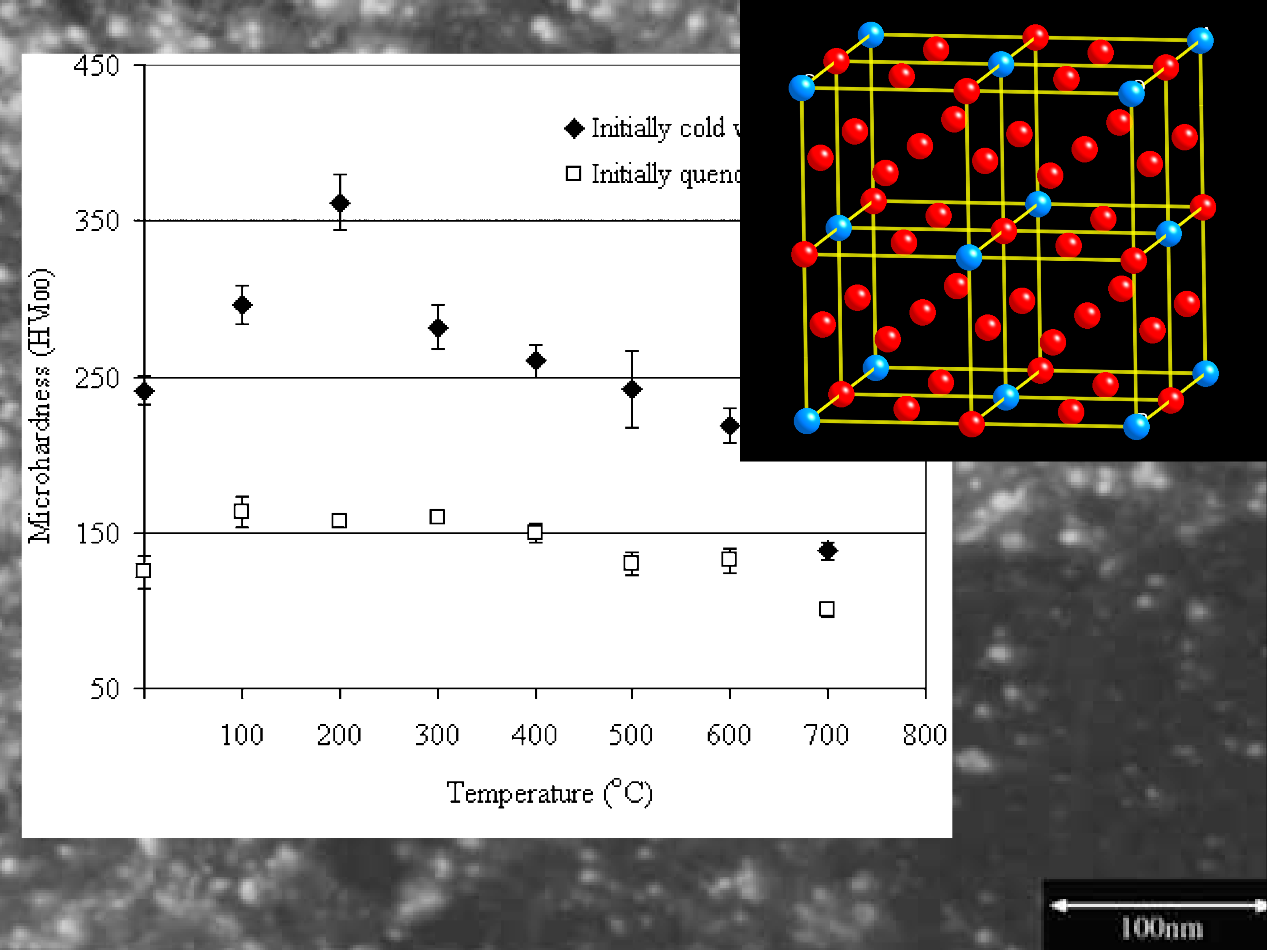
But I want to explore a larger space...and go to finite T...


PLATINUM
9995
1 OUNCE TROY

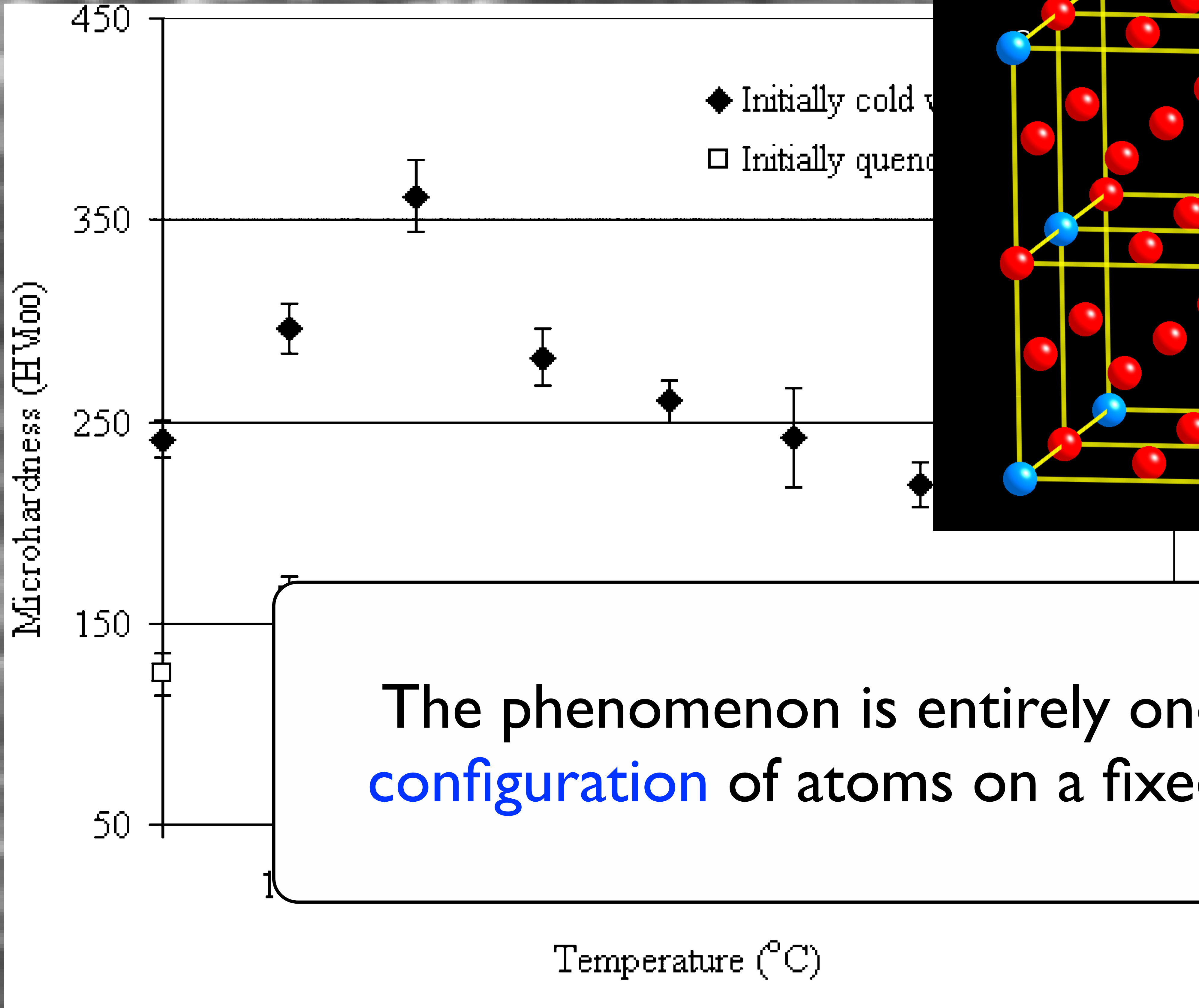

1 OUNCE TROY

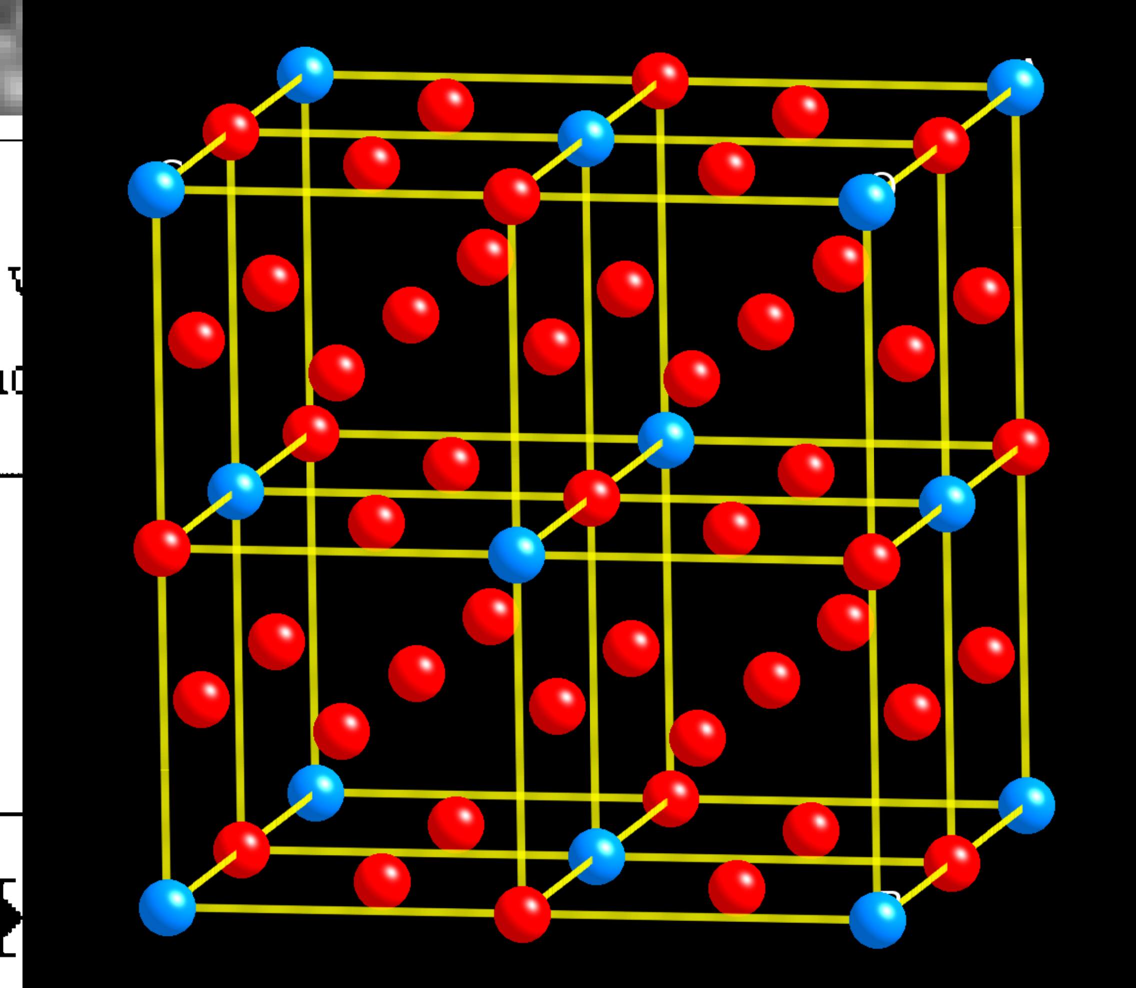

100nm

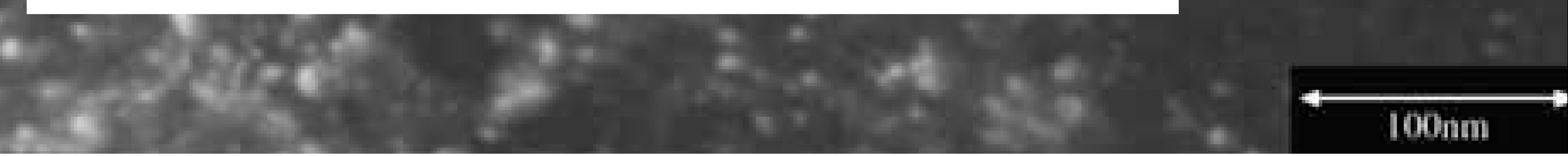

100nm



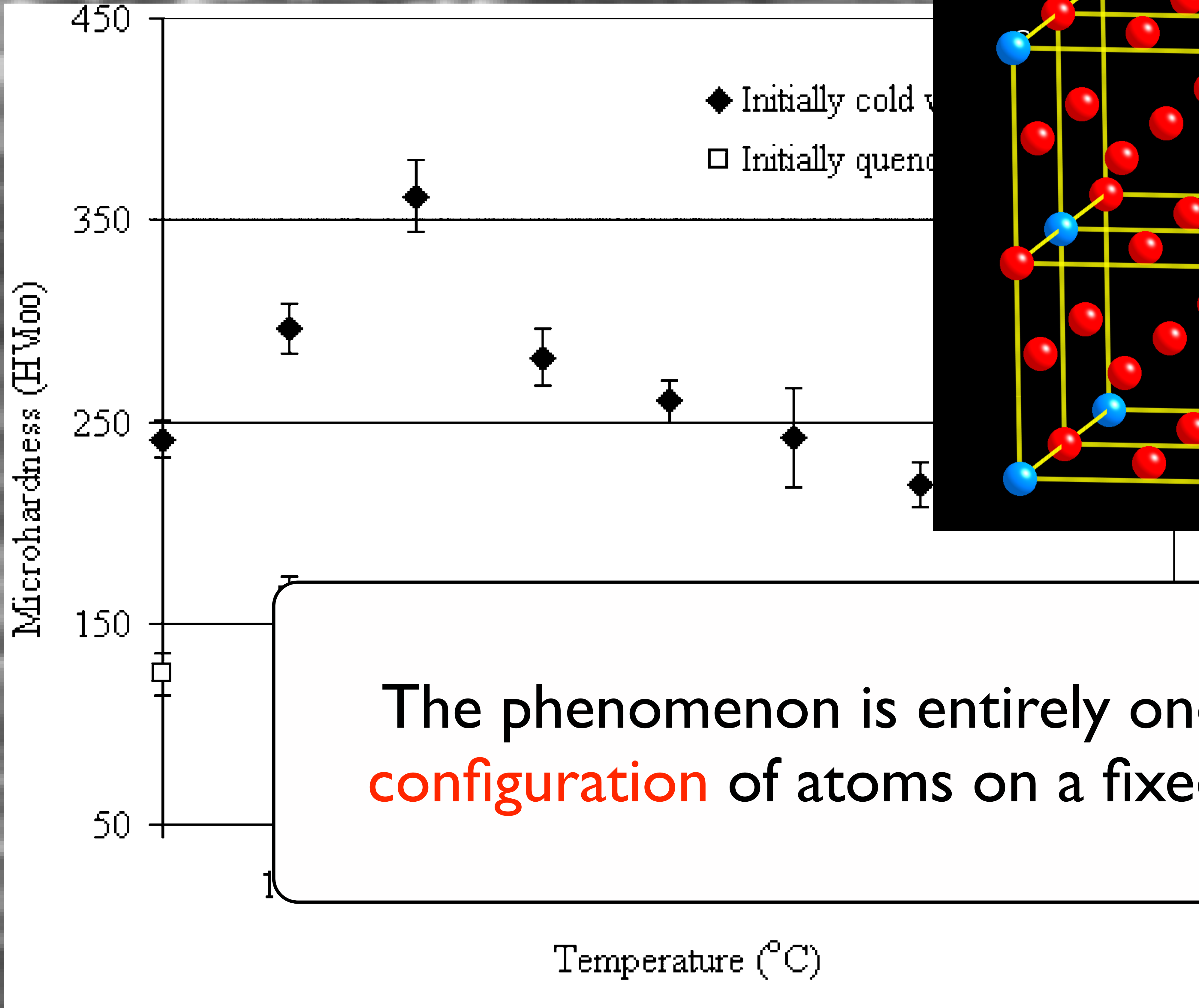
Initially cold w
Initially quenc
Microhardness (HV100)
450
350
250
150
50
100
200
300
400
500
600
700
800
Temperature (°C)
100nm

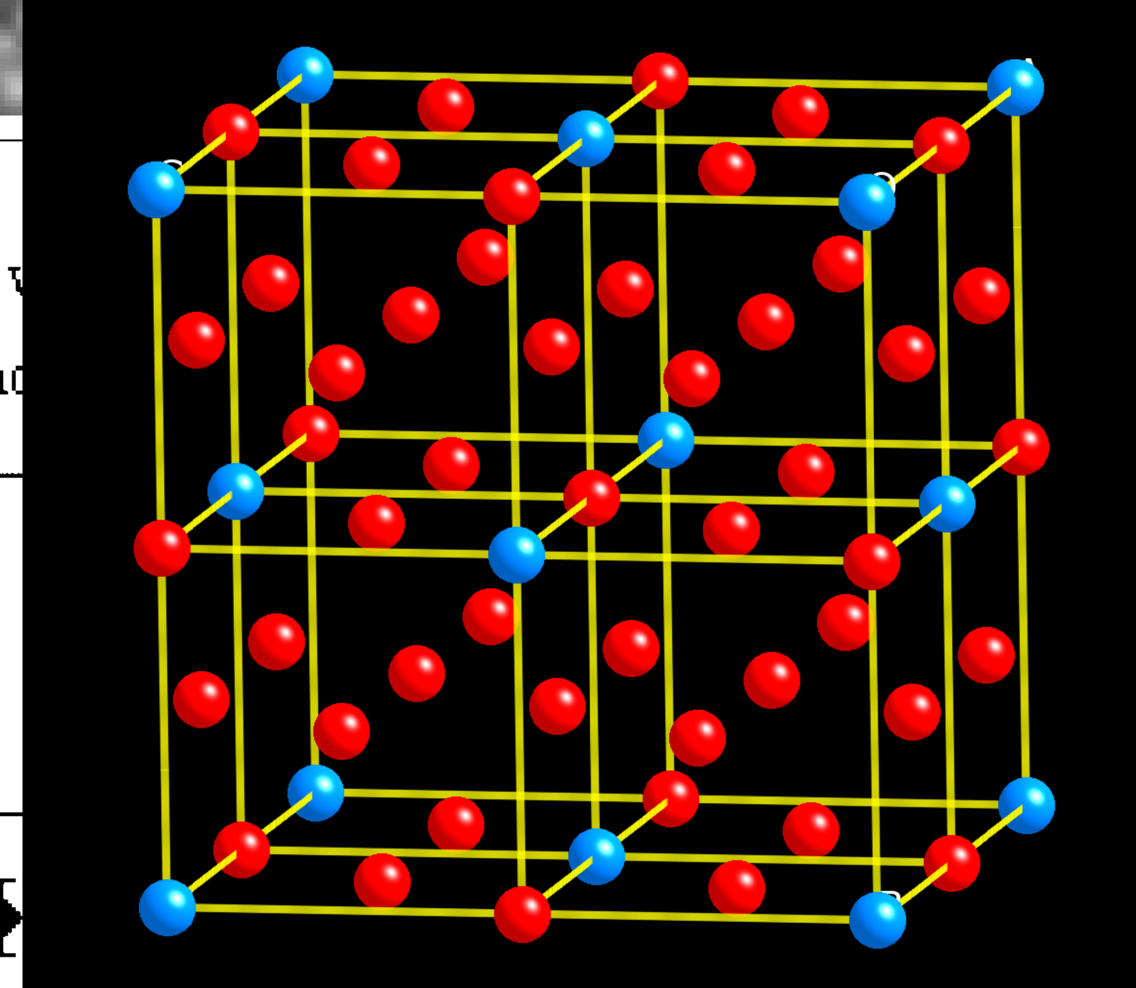






The phenomenon is entirely one of the configuration of atoms on a fixed lattice.

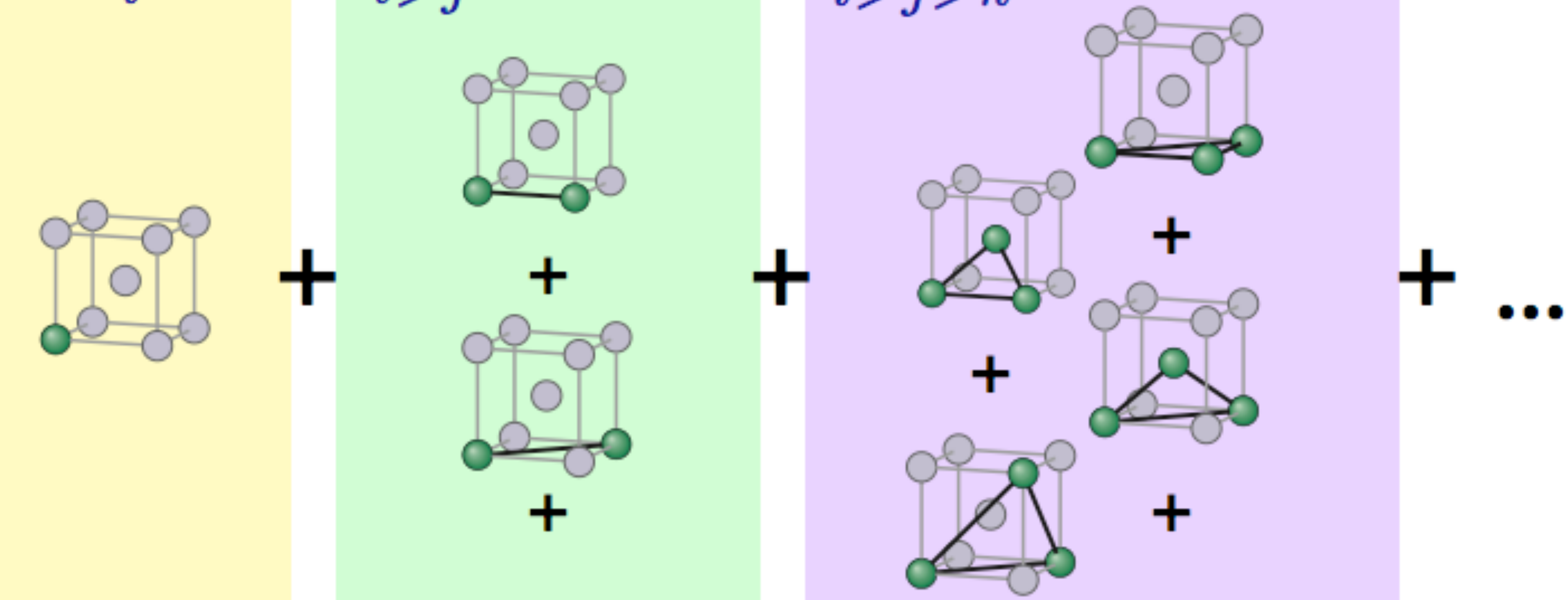


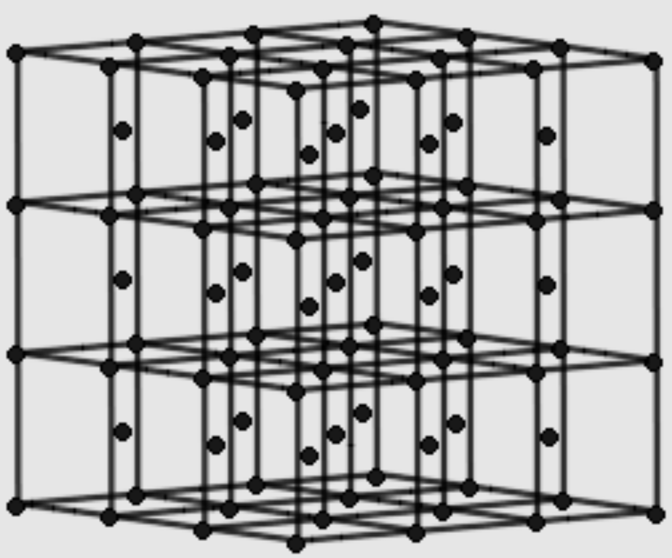


The phenomenon is entirely one of the configuration of atoms on a fixed lattice.

$$\Lambda(\vec{\sigma}) = J_0 + J_1 \sum_i \sigma_i + \sum_{i>j} J_{ij}\sigma_i\sigma_j + \sum_{i>j>k} J_{ijk}\sigma_i\sigma_j\sigma_k + \cdots$$

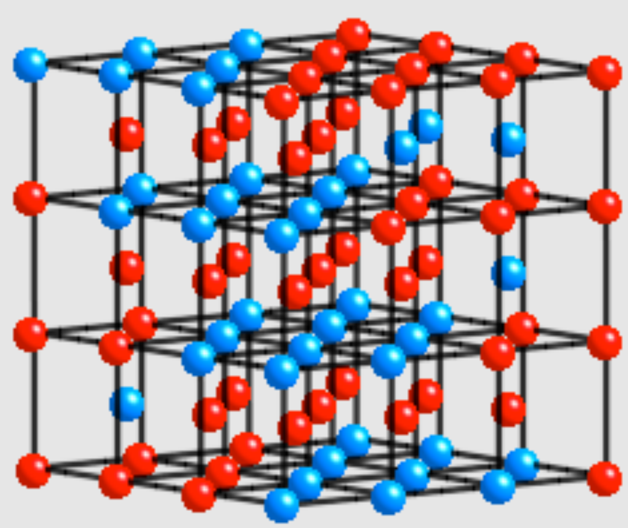
$\Lambda =$



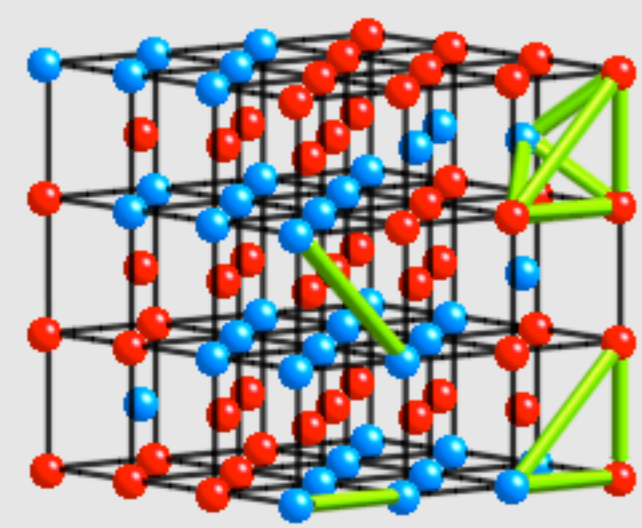


Basic Lattice

Configuration: $\vec{\sigma}$

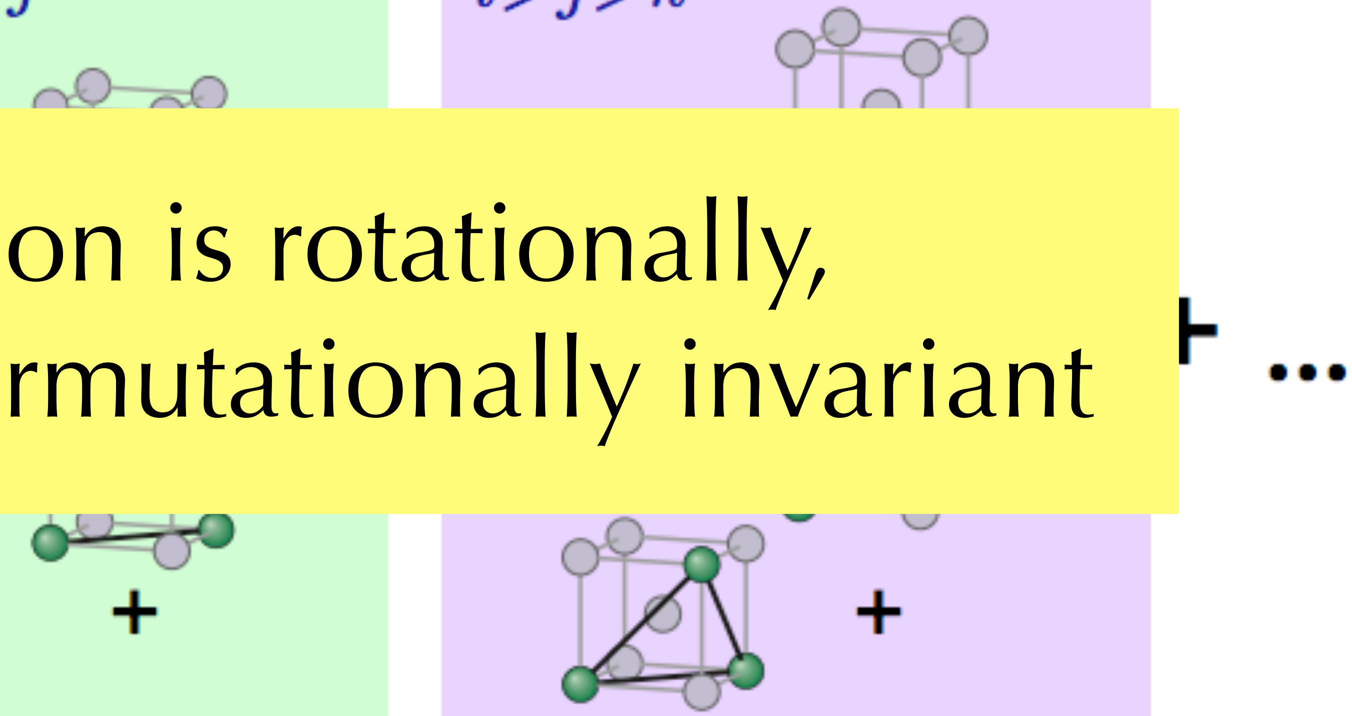


$\sigma_n = \pm 1$ (A or B)

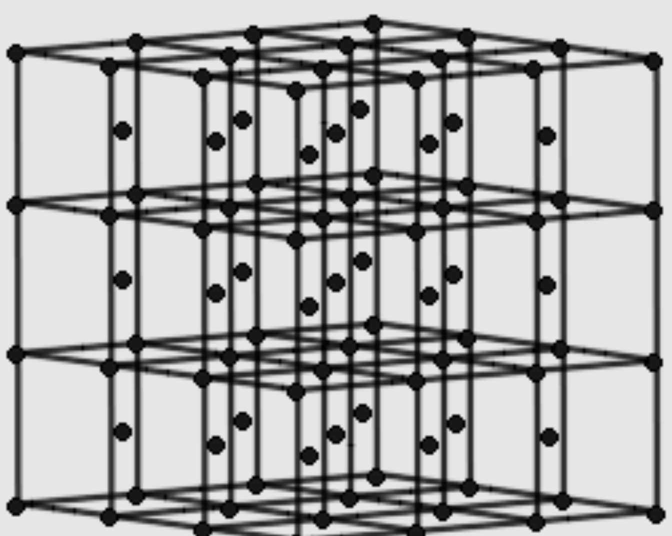


Interactions

$$\Lambda(\vec{\sigma}) = J_0 + J_1 \sum_i \sigma_i + \sum_{i>j} J_{ij}\sigma_i\sigma_j + \sum_{i>j>k} J_{ijk}\sigma_i\sigma_j\sigma_k + \cdots$$



Representation is rotationally, translationally, permutationally invariant



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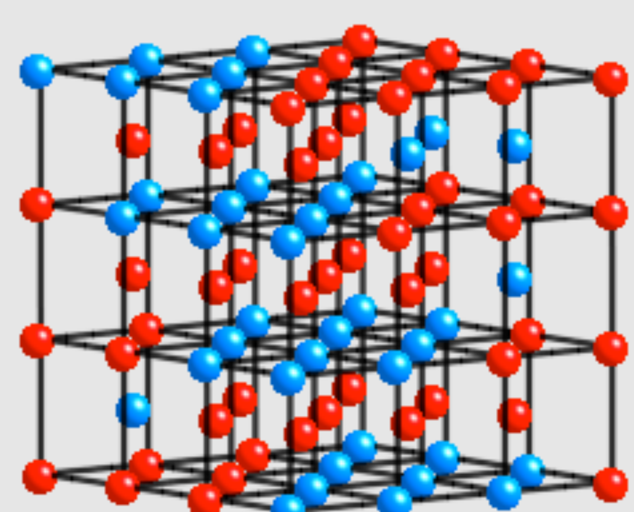

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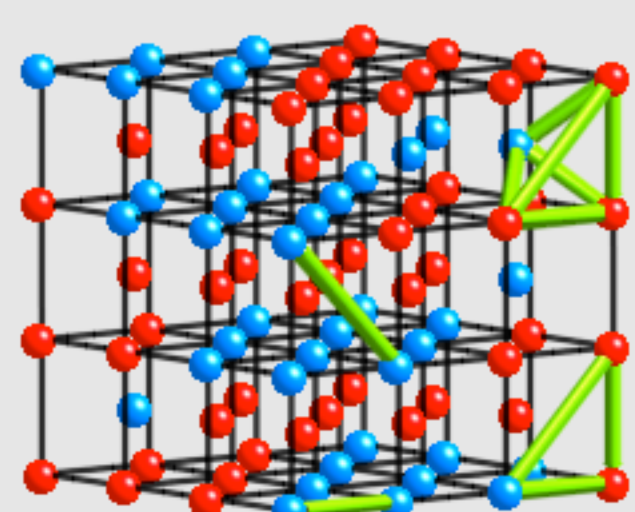
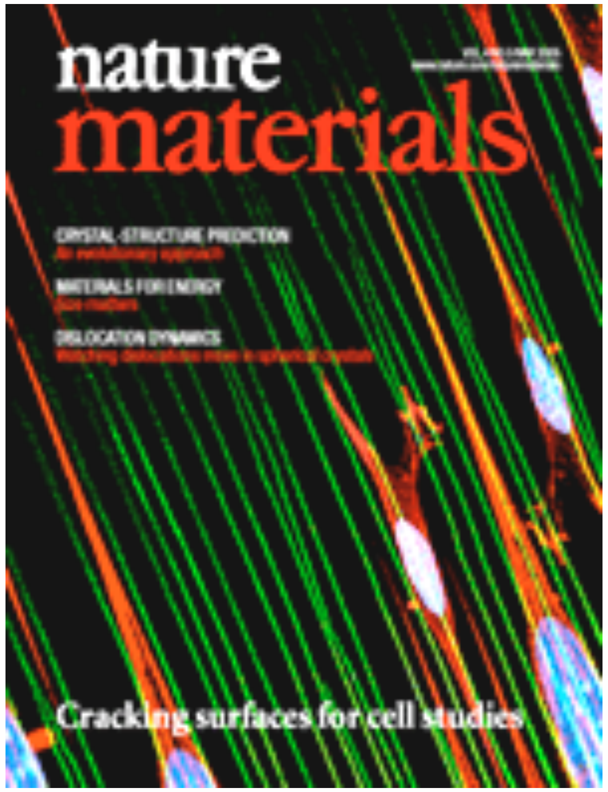
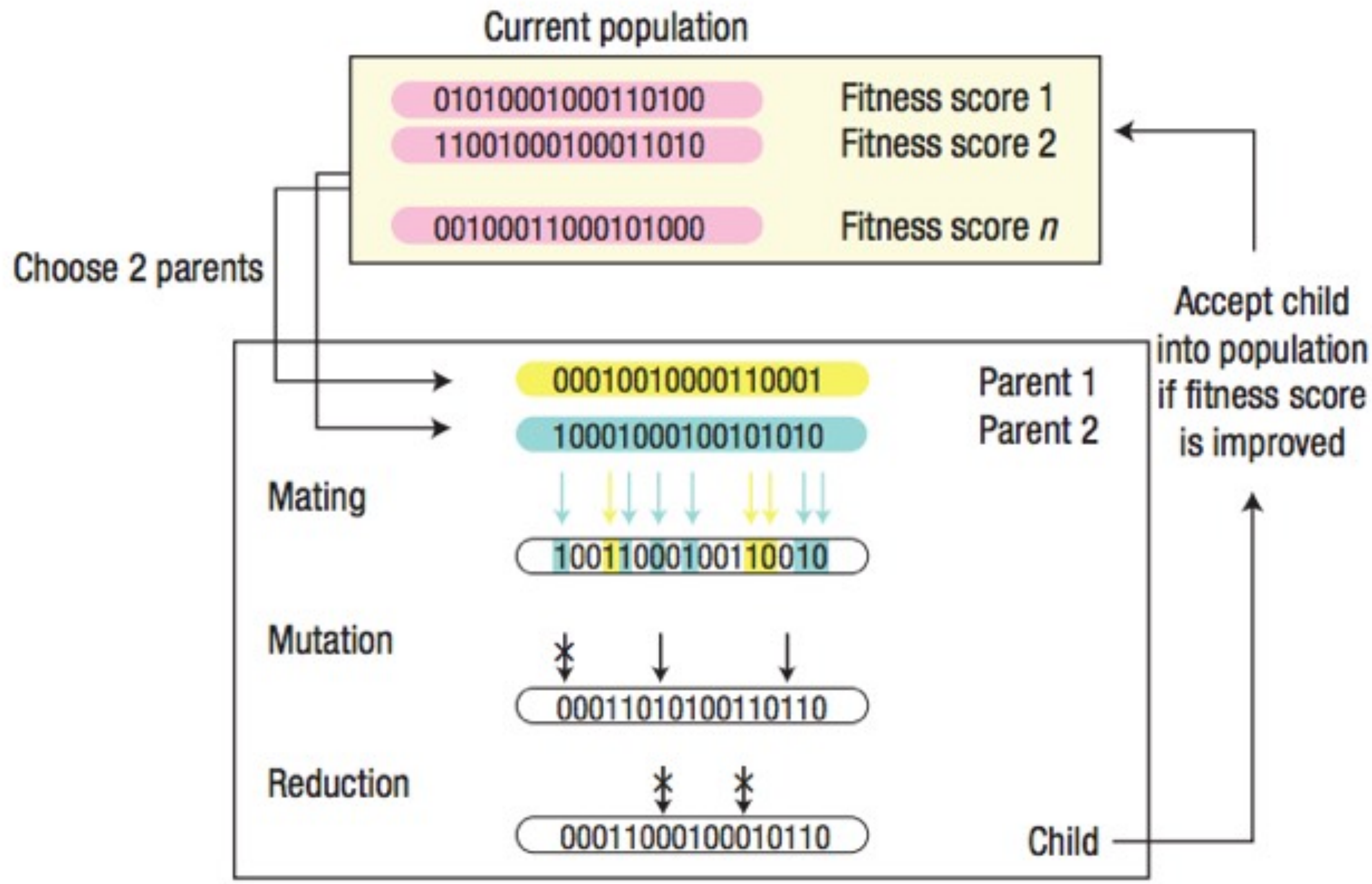


Interactions

Genetic Algorithm for Model Building





LETTERS

Evolutionary approach for determining first-principles hamiltonians

GUS L. W. HART[1]*, VOLKER BLUM[2]†, MICHAEL J. WALORSKI[3] AND ALEX ZUNGER[2]

[1]Department of Physics and Astronomy, Northern Arizona University, Flagstaff, Arizona 86011-6010, USA

[2]National Renewable Energy Laboratory, Golden, Colorado 80401, USA

"Solving" an under-determined problem

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$$\mathbb{M}\vec{a} = \vec{f}$$

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$$\min_{\vec{a}} \left\{ \|\vec{a}\|_1 : \mathbb{M}\vec{a} = \vec{f} \right\}$$

“Solving” an under-determined problem

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$$\ell_1 \equiv \|\vec{u}\| = \sum_i |u_i|$$

"Solving" an under-determined problem

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$$\ell_1 \equiv \|\vec{u}\| = \sum_i |u_i|$$

$$\ell_2 \equiv \left(\sum_i |u_i|^2 \right)^{\frac{1}{2}} \qquad \ell_1 \equiv \left(\sum_i |u_i|^1 \right)^{\frac{1}{1}}$$

Practicality of CS: ℓ_1 norm techniques

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CS is practical because there are so many good numerical approaches for enforcing the ℓ_1 norm

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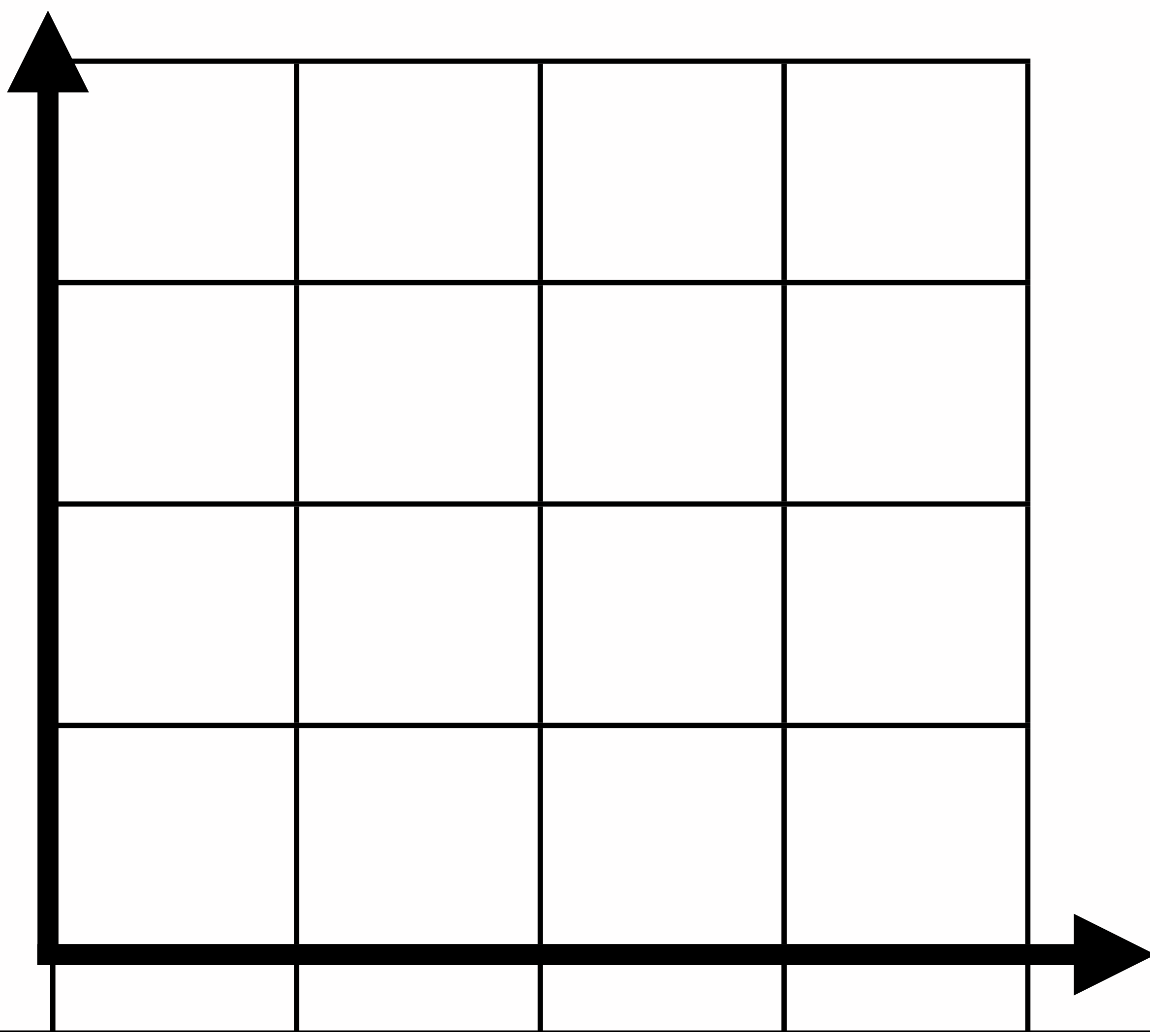

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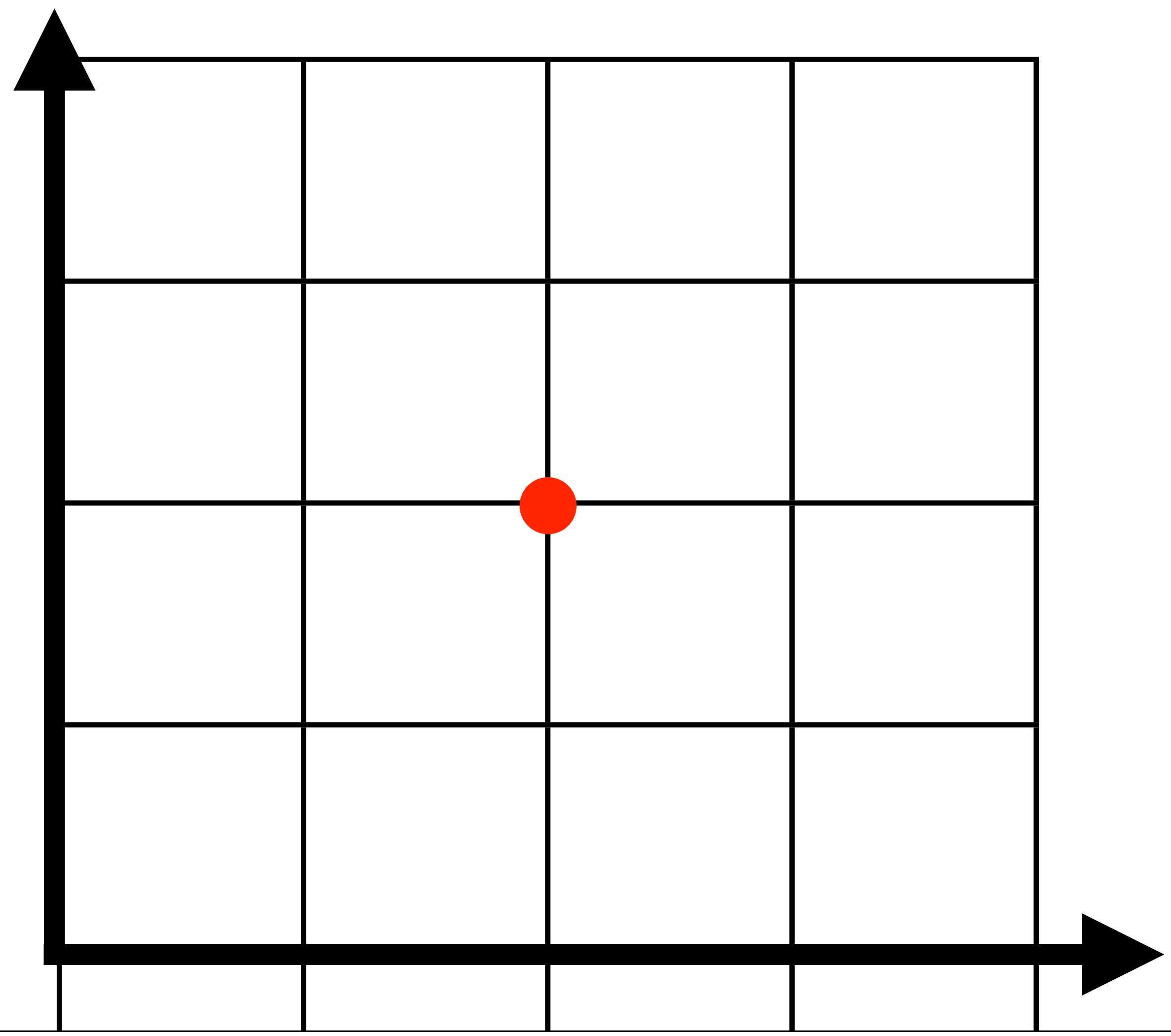

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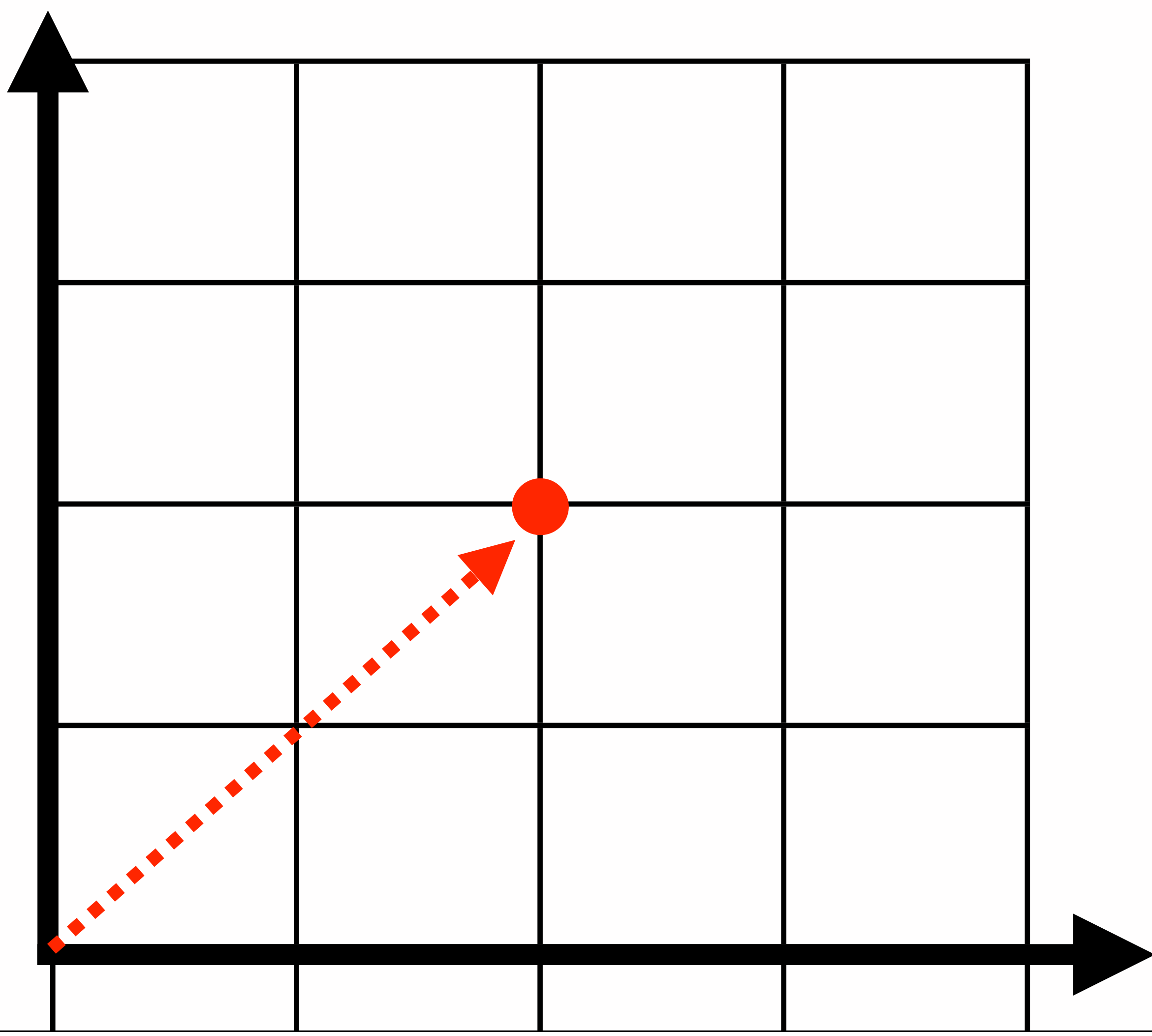

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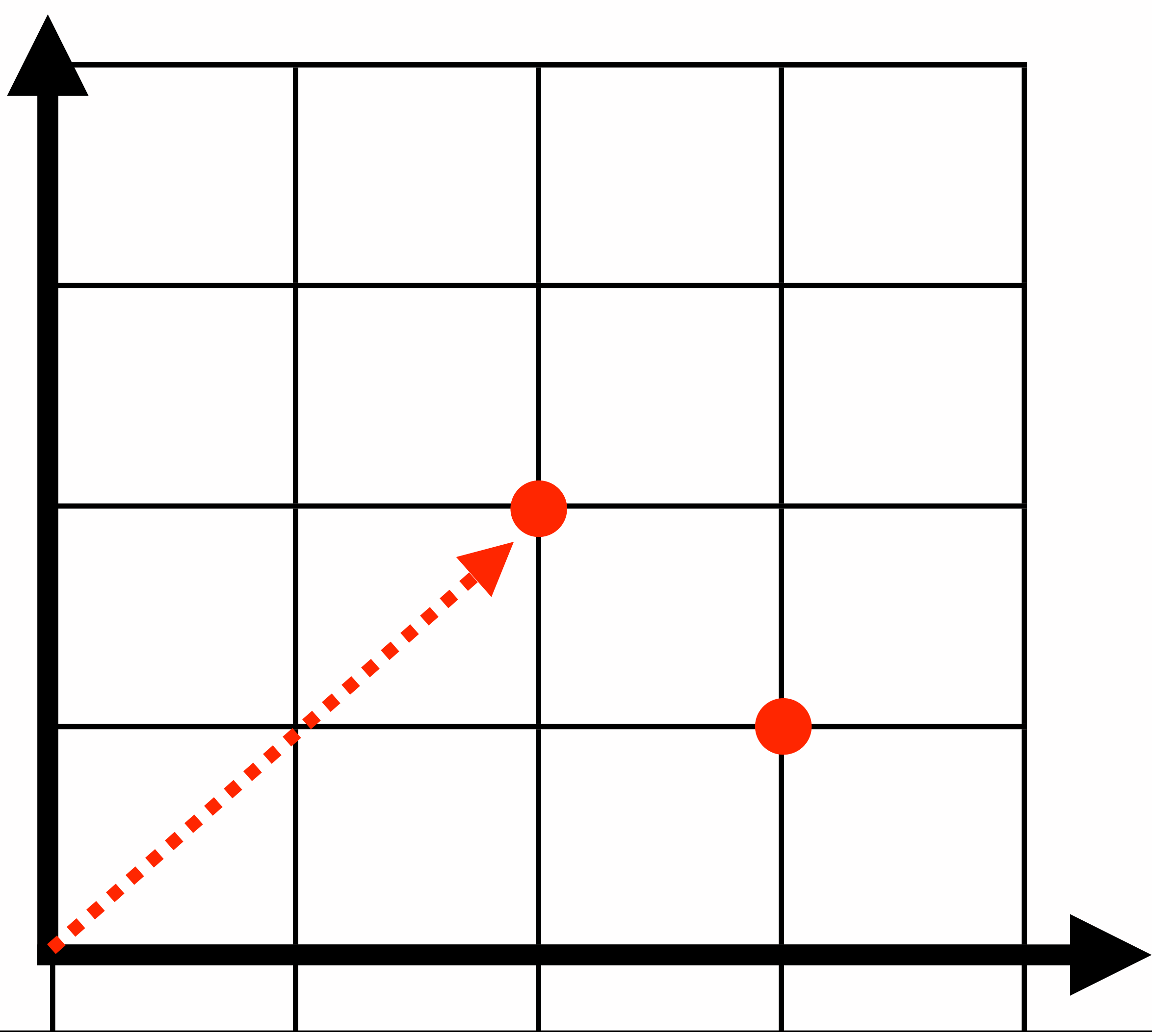

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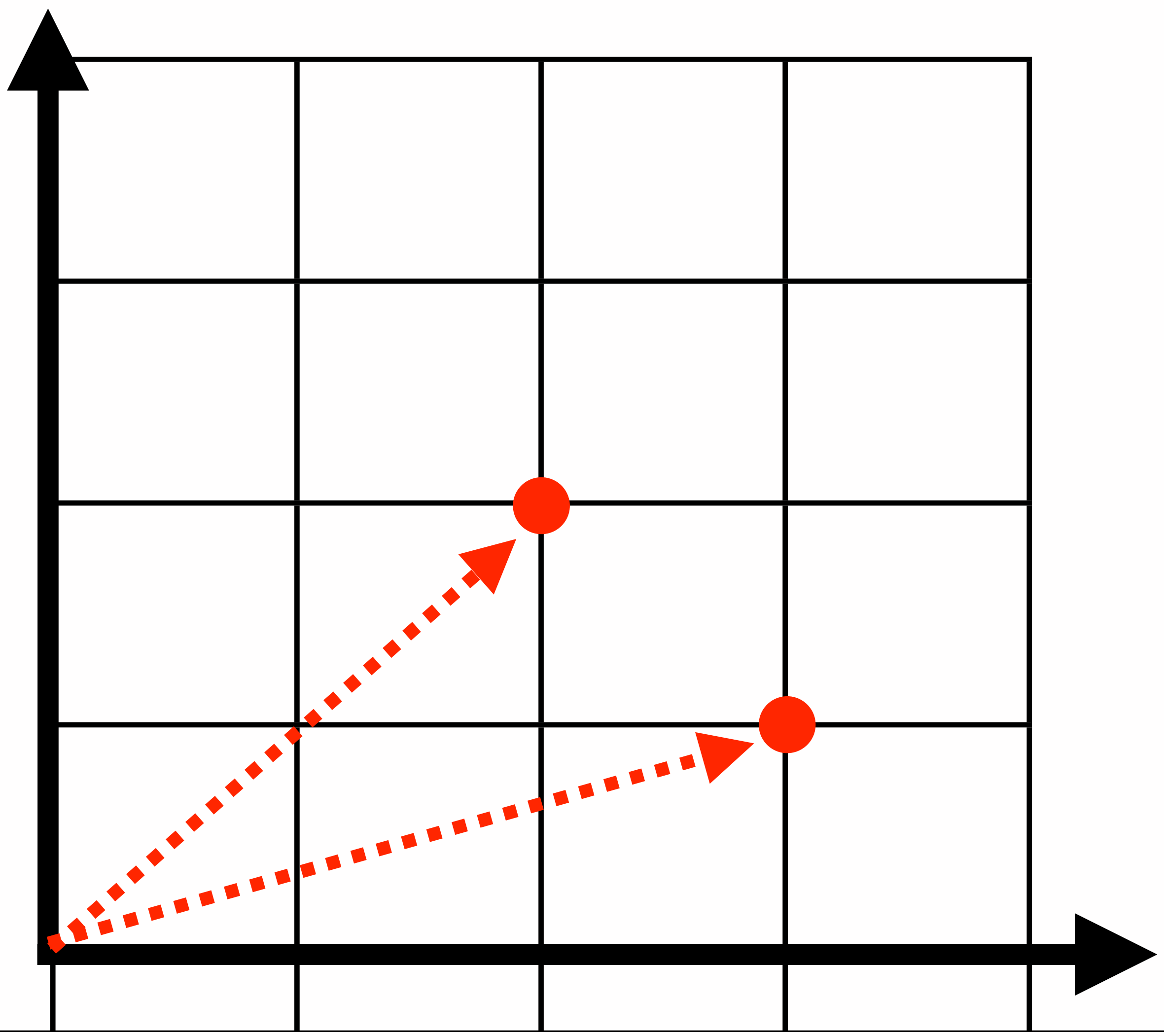

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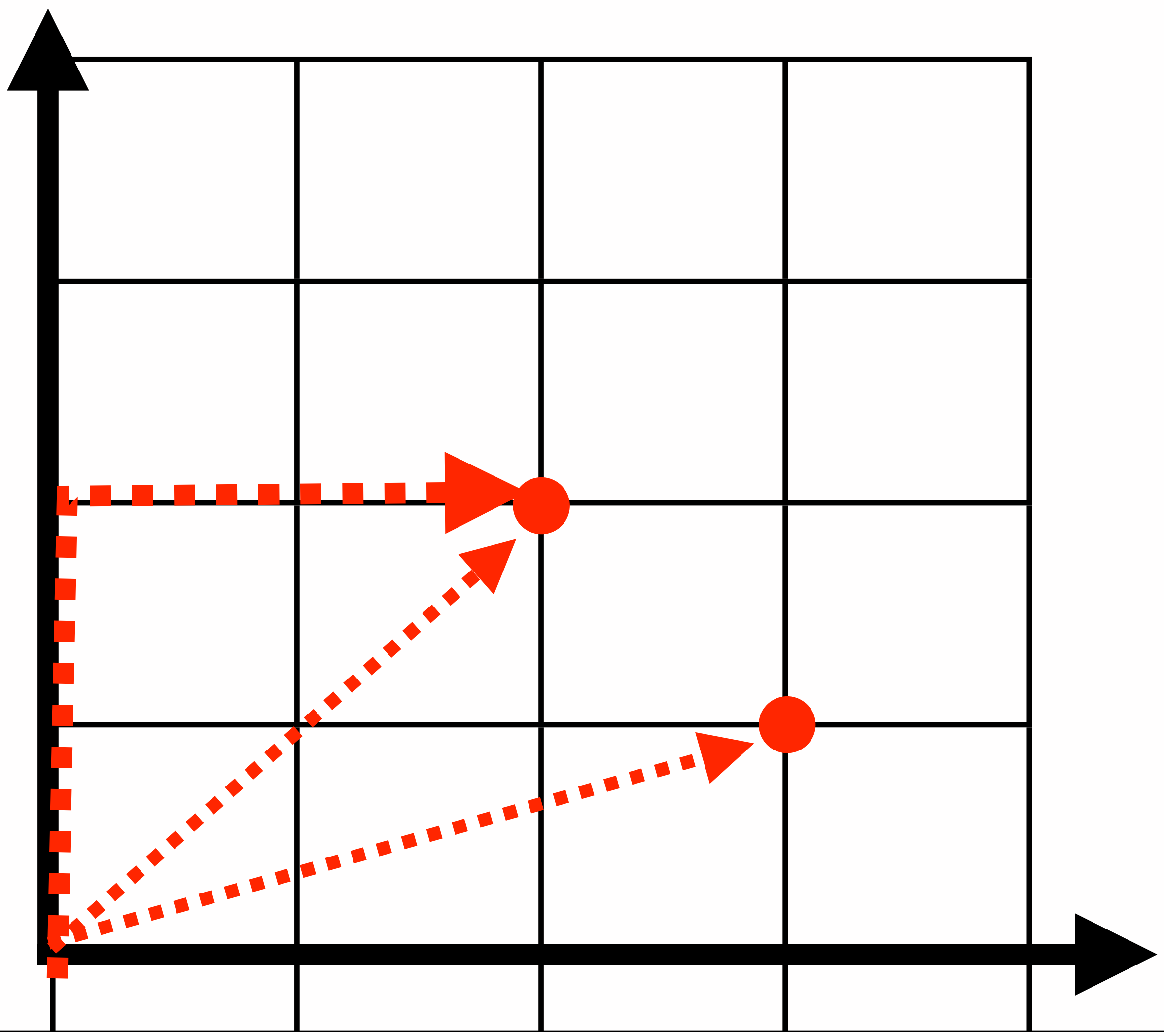

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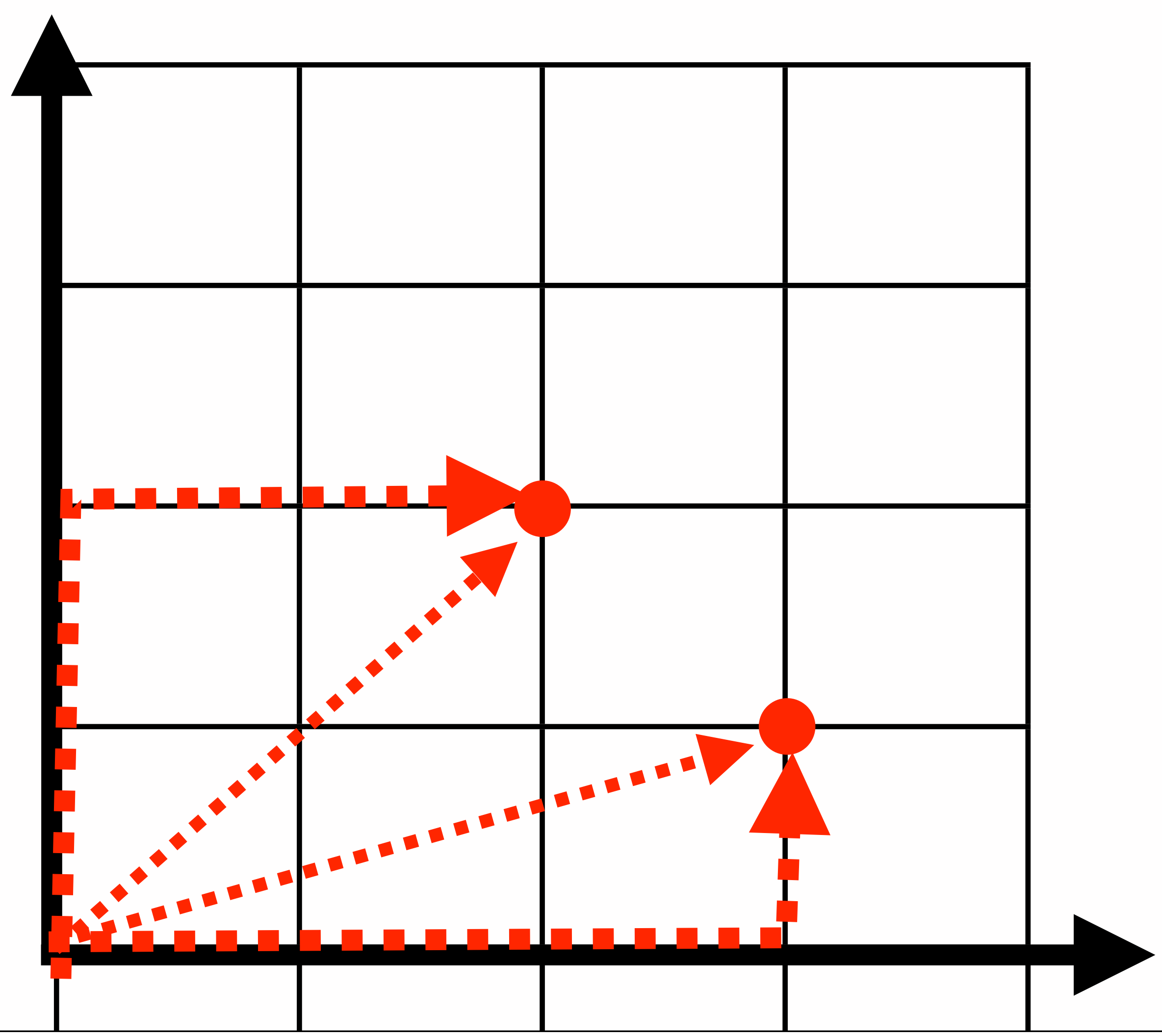

Practicality of CS: ℓ_1 norm techniques

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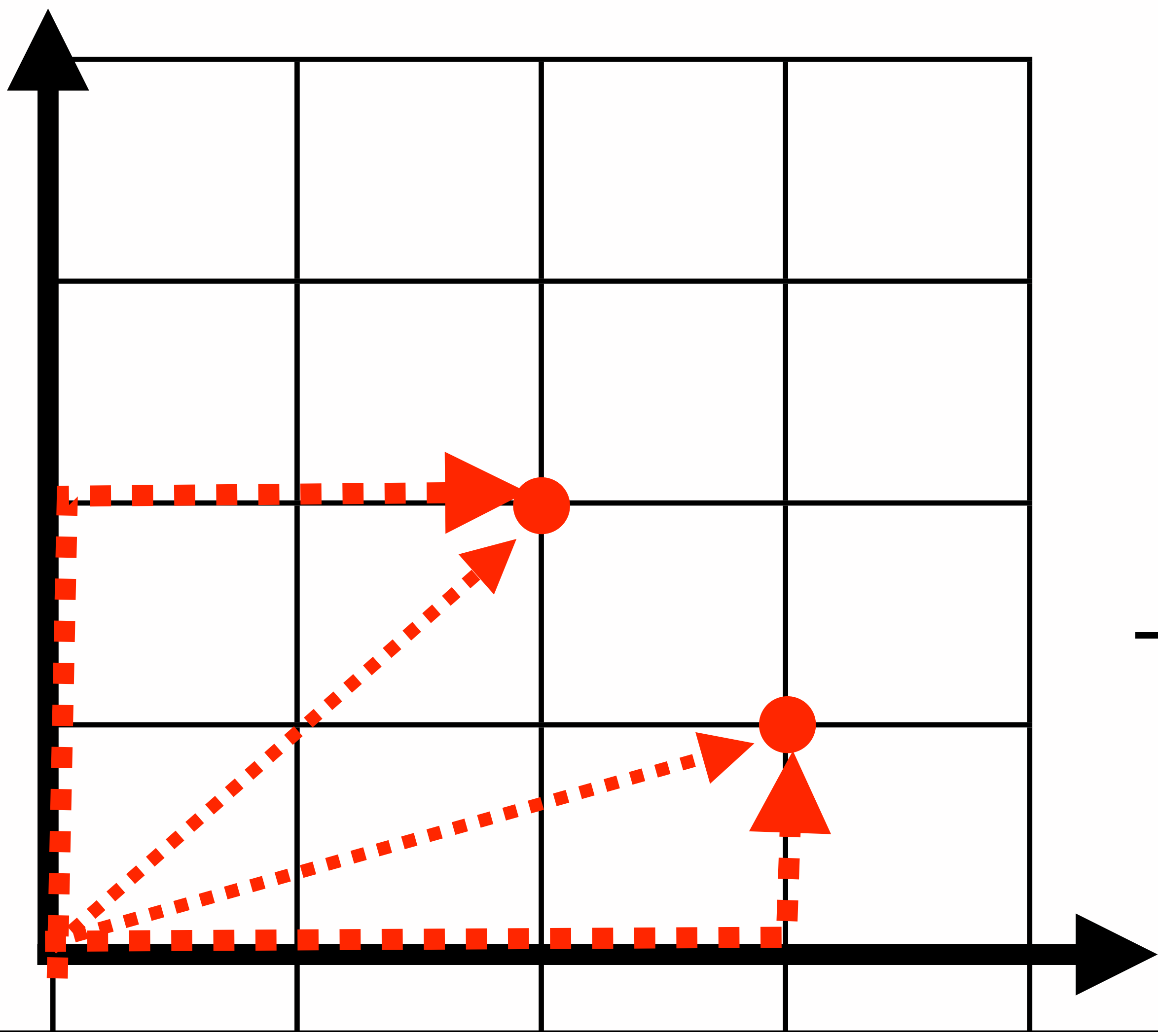
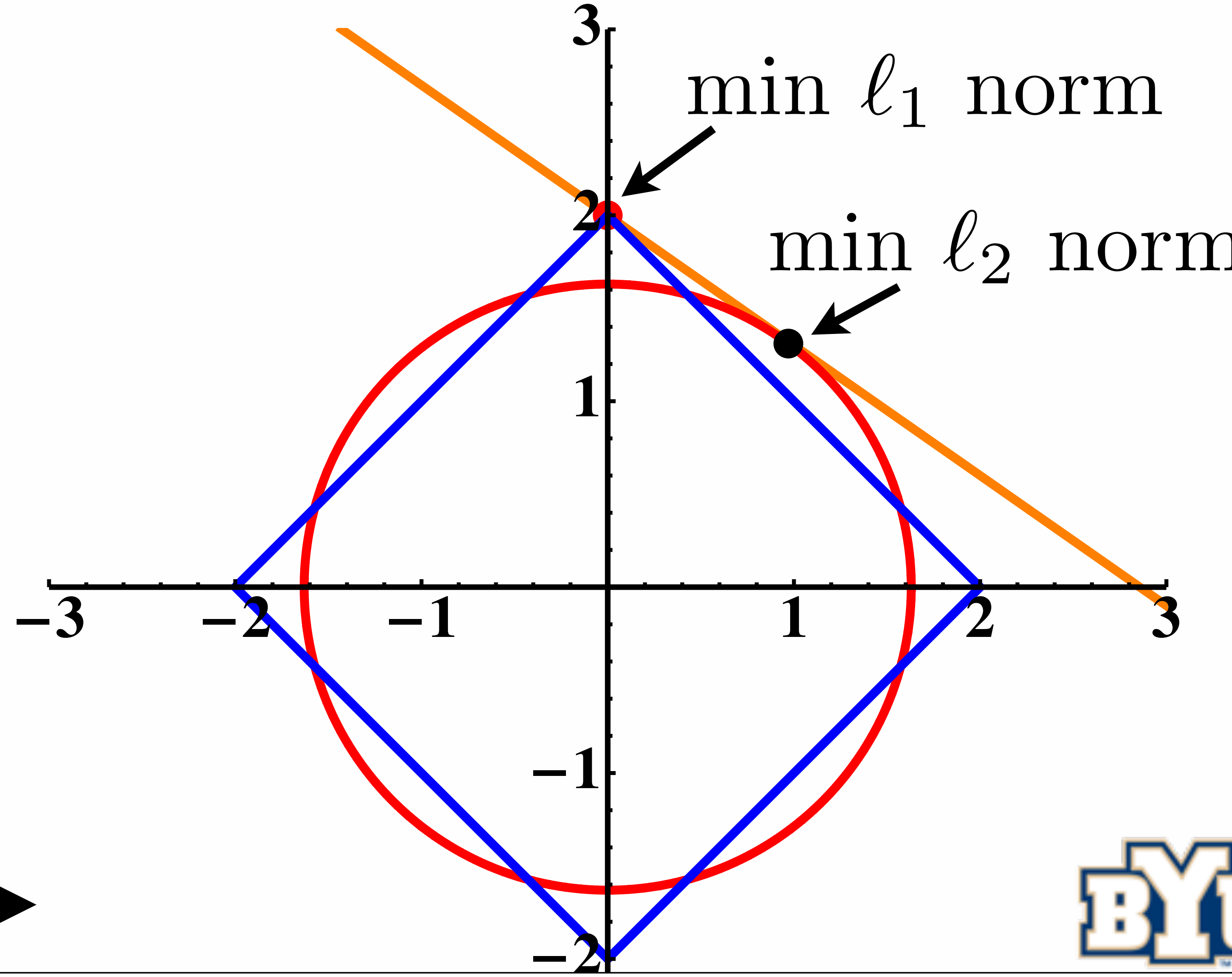
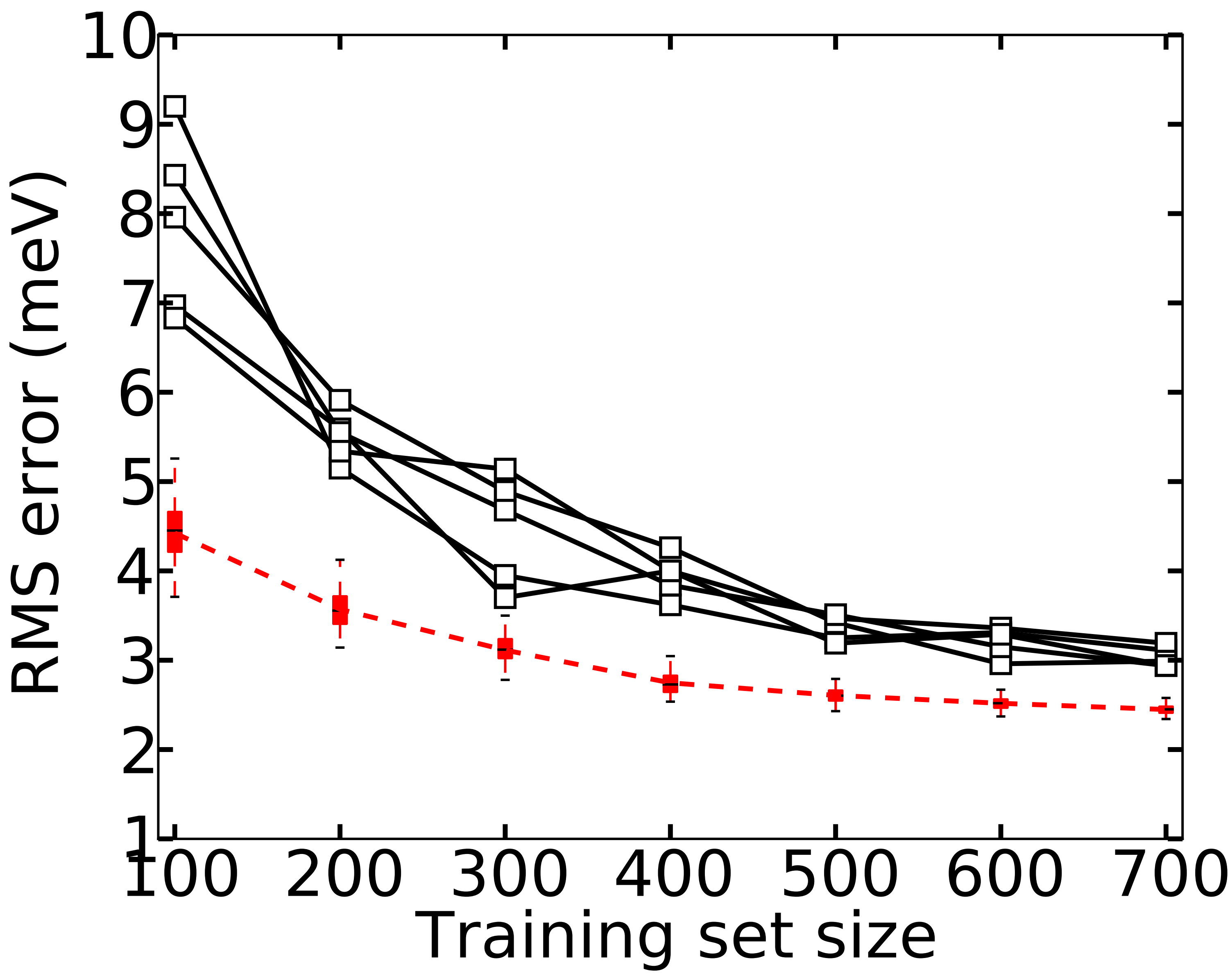




Bayesian Compressive Sensing vs. GA



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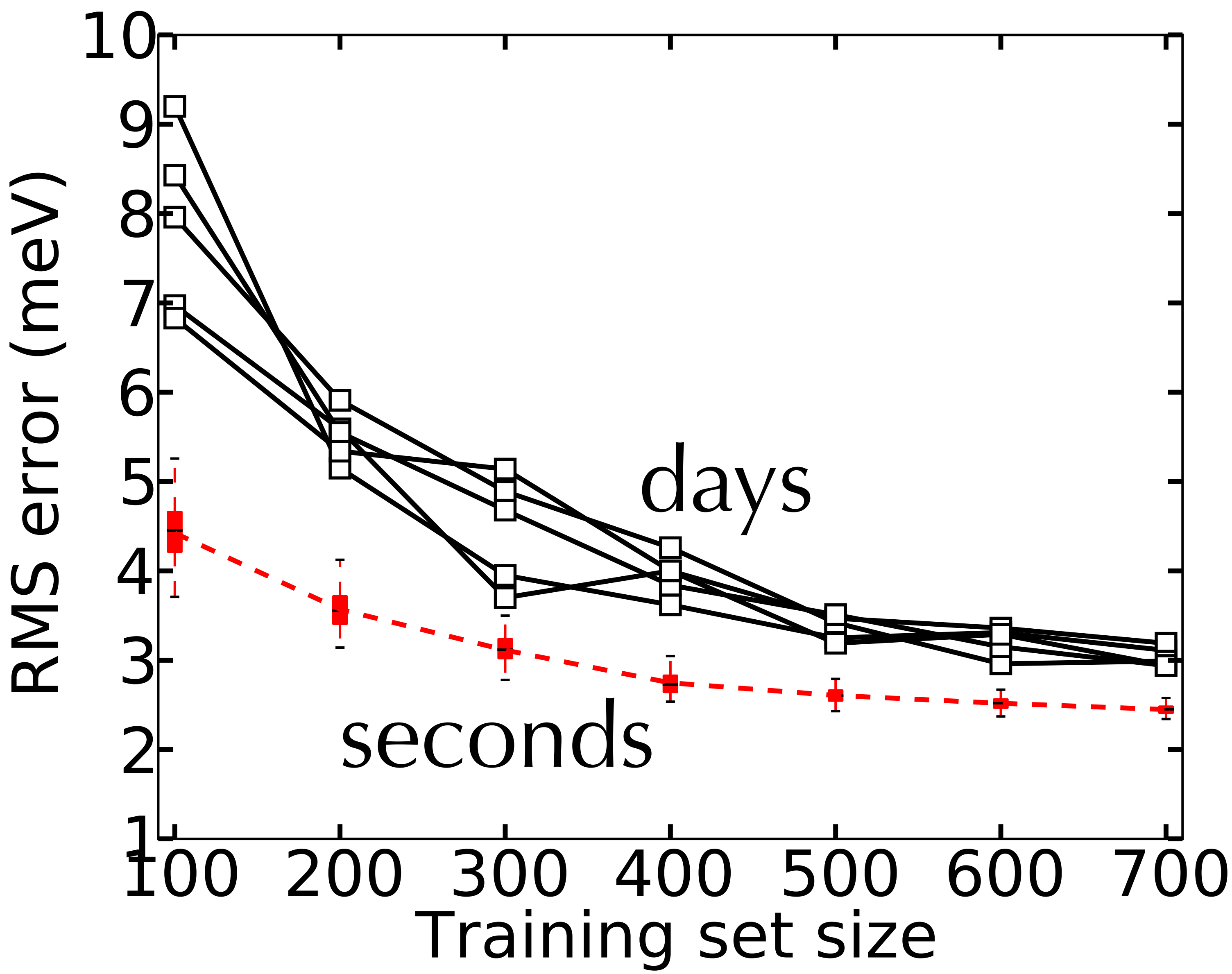

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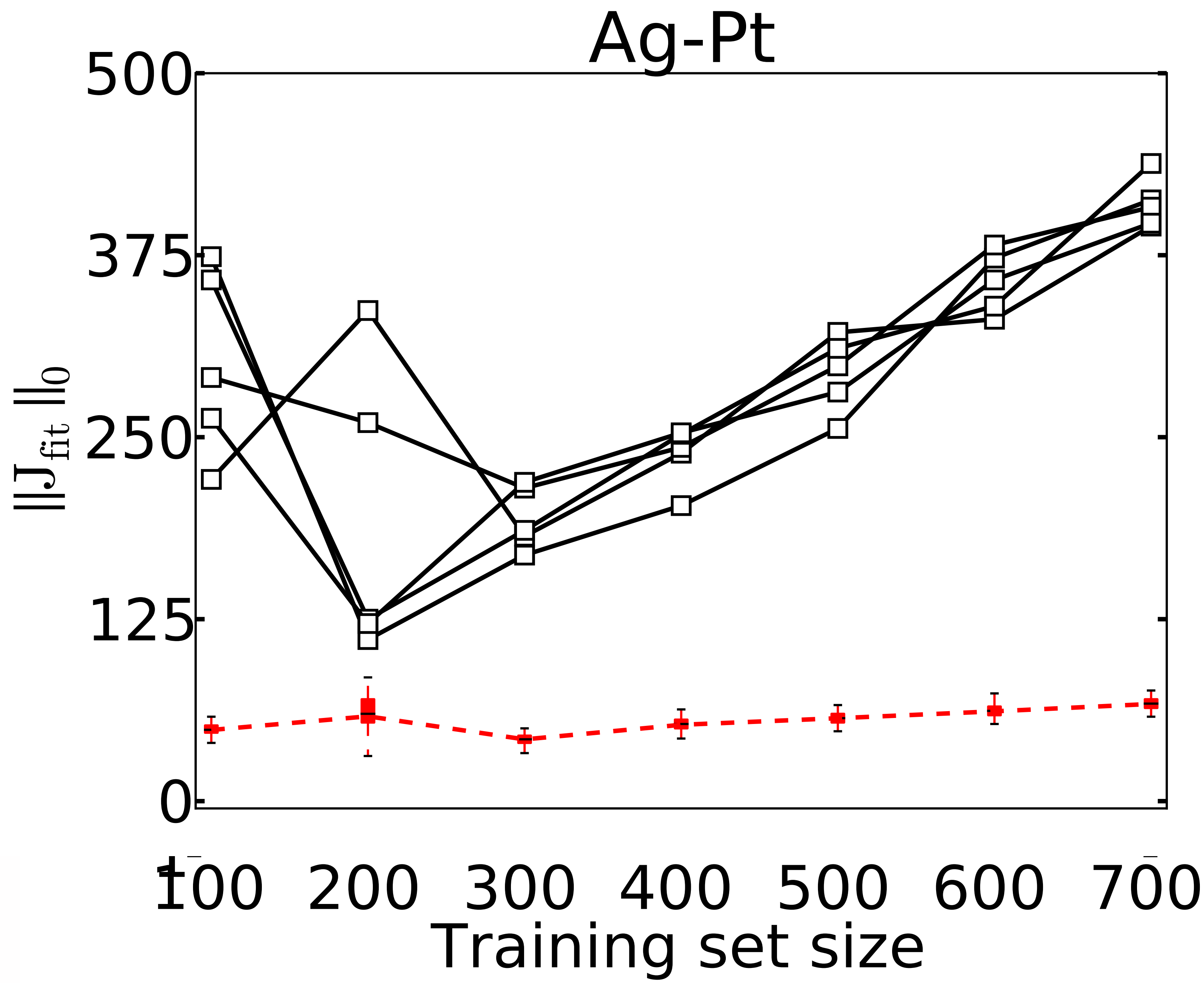
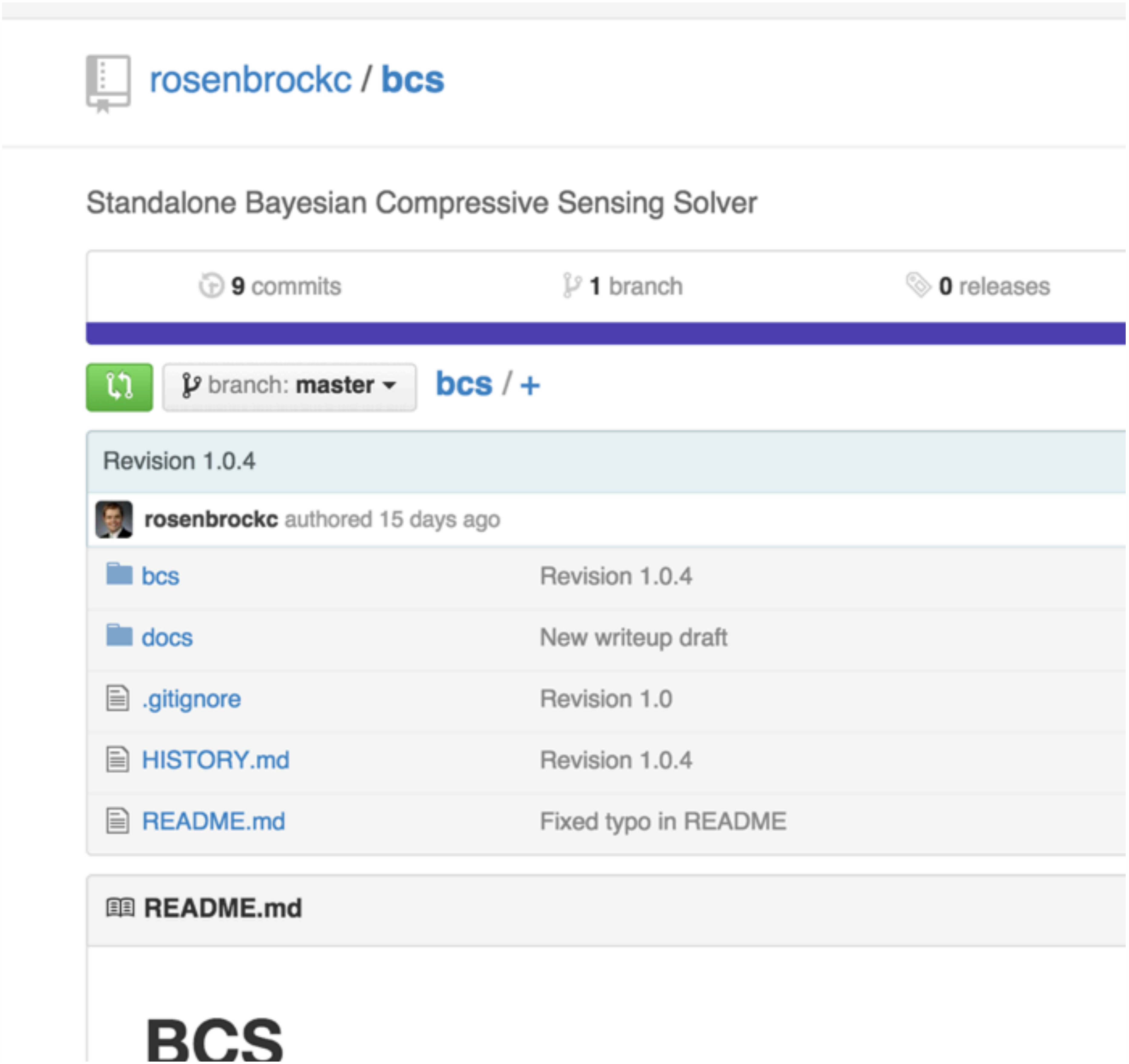


Bayesian Compressive Sensing Stand-alone Solver



But I want to explore a ***much*** larger space…and go to finite T…

But I want to explore a ***much*** larger space…and go to finite T…

I′d like to go off the lattice…

But compressive sensing uncovered DFT problems

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$$\int_0^1 (x - 1/2)^2 \, dx$$

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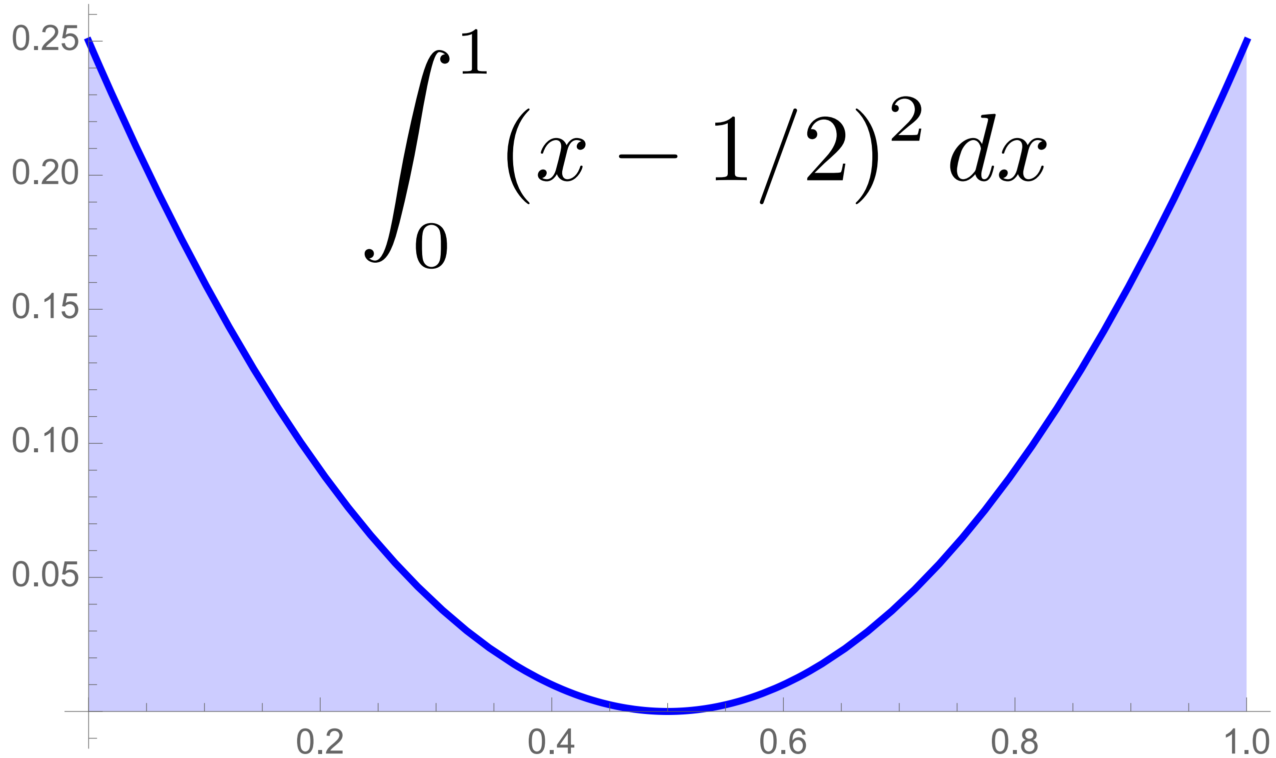

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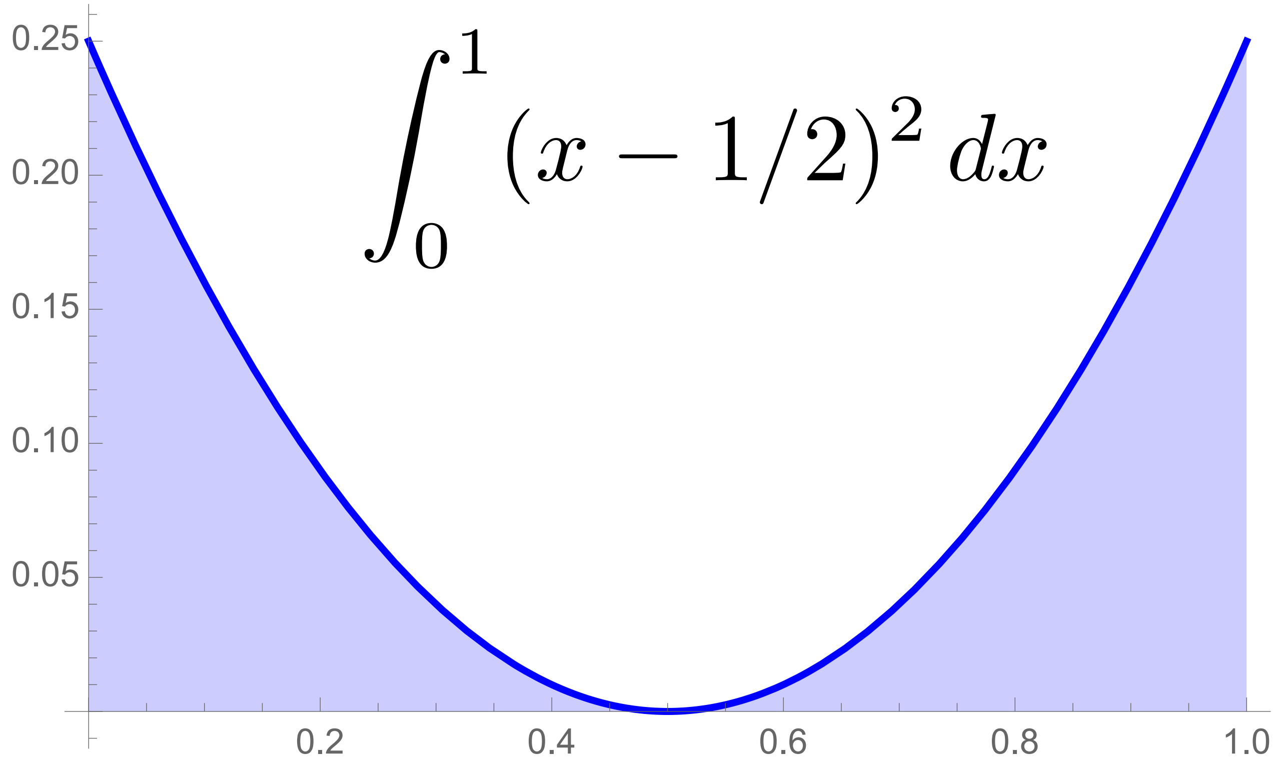

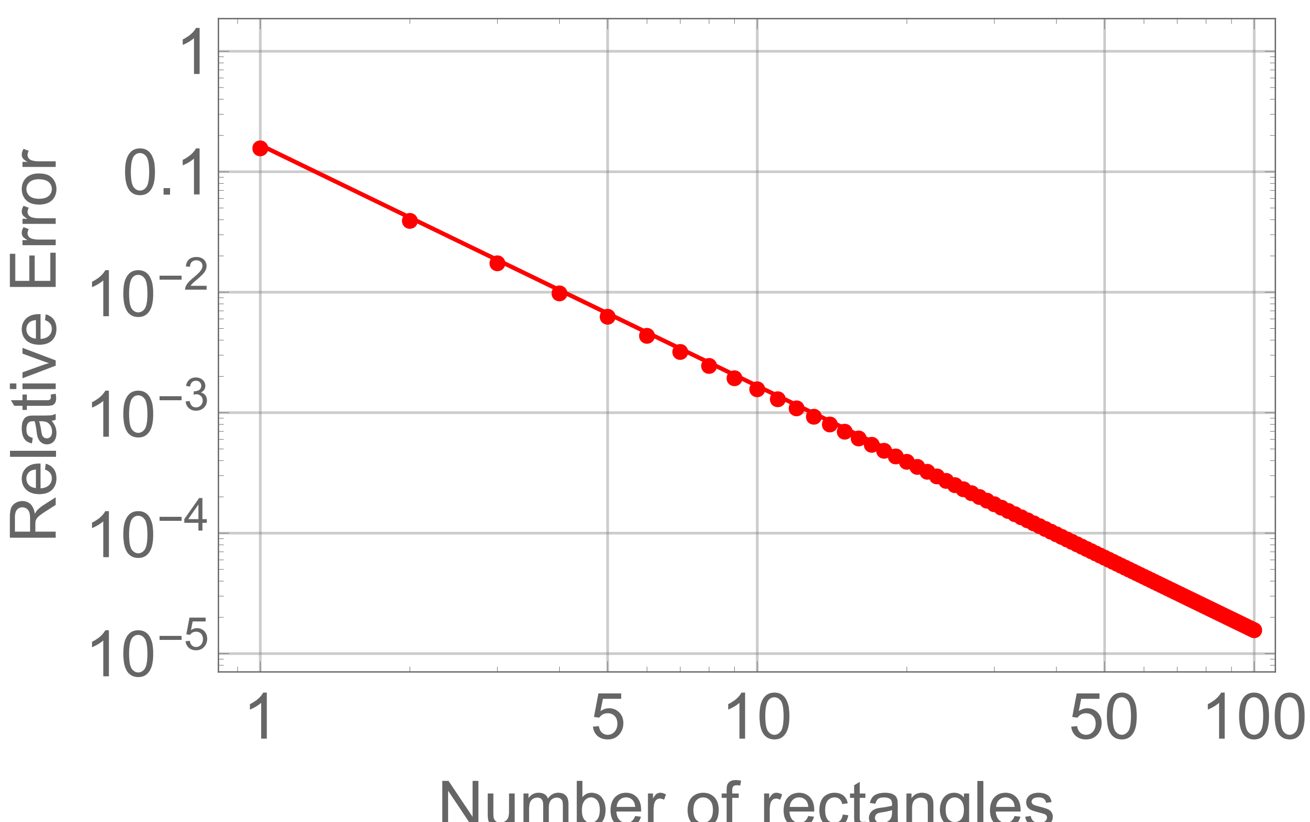

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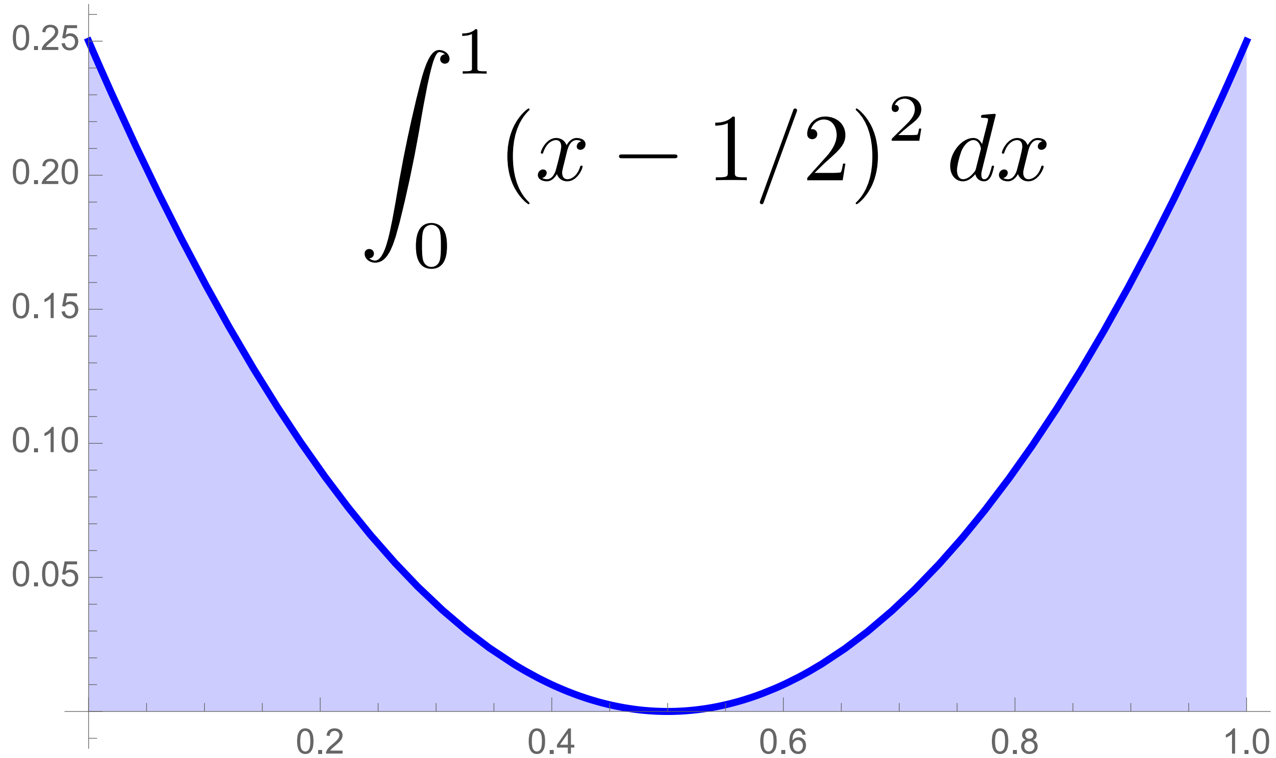

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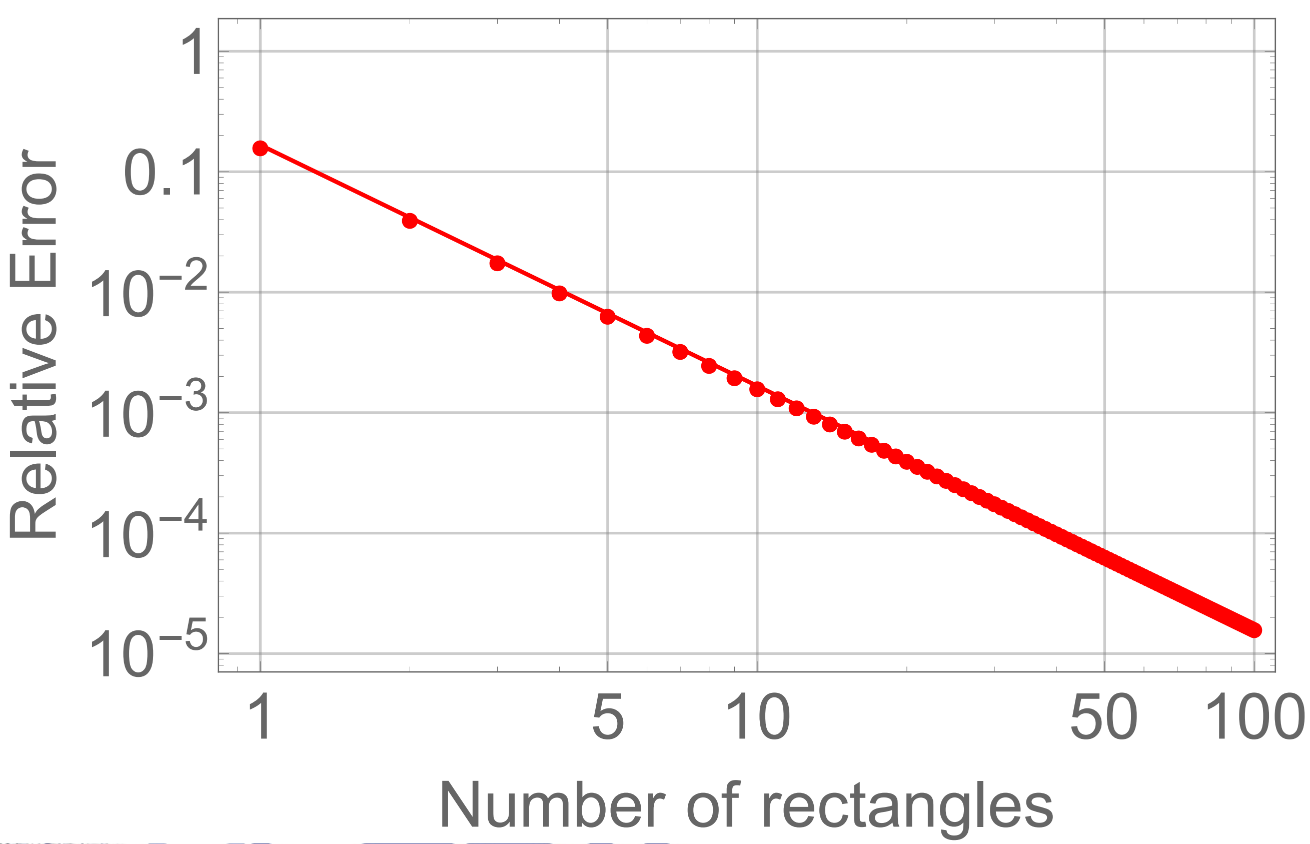

$$\int_0^1 e^{\cos 2\pi x} \, dx$$

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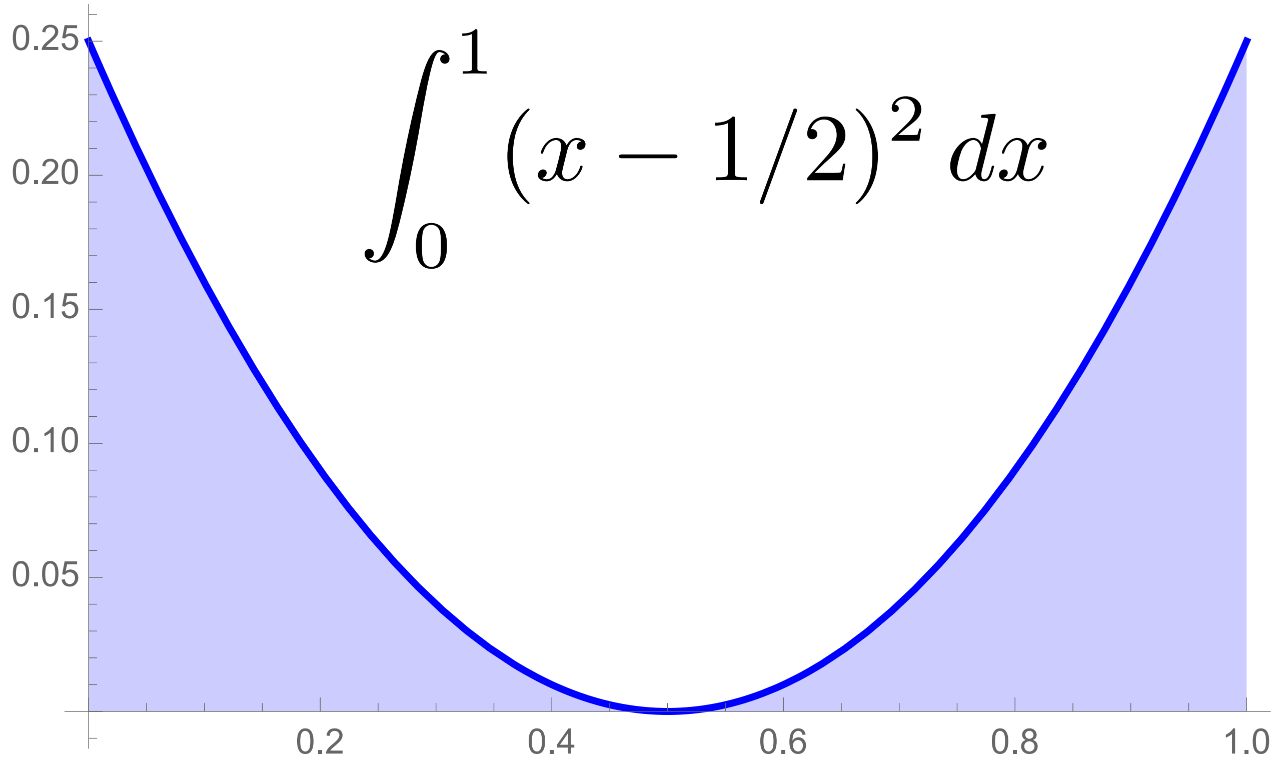

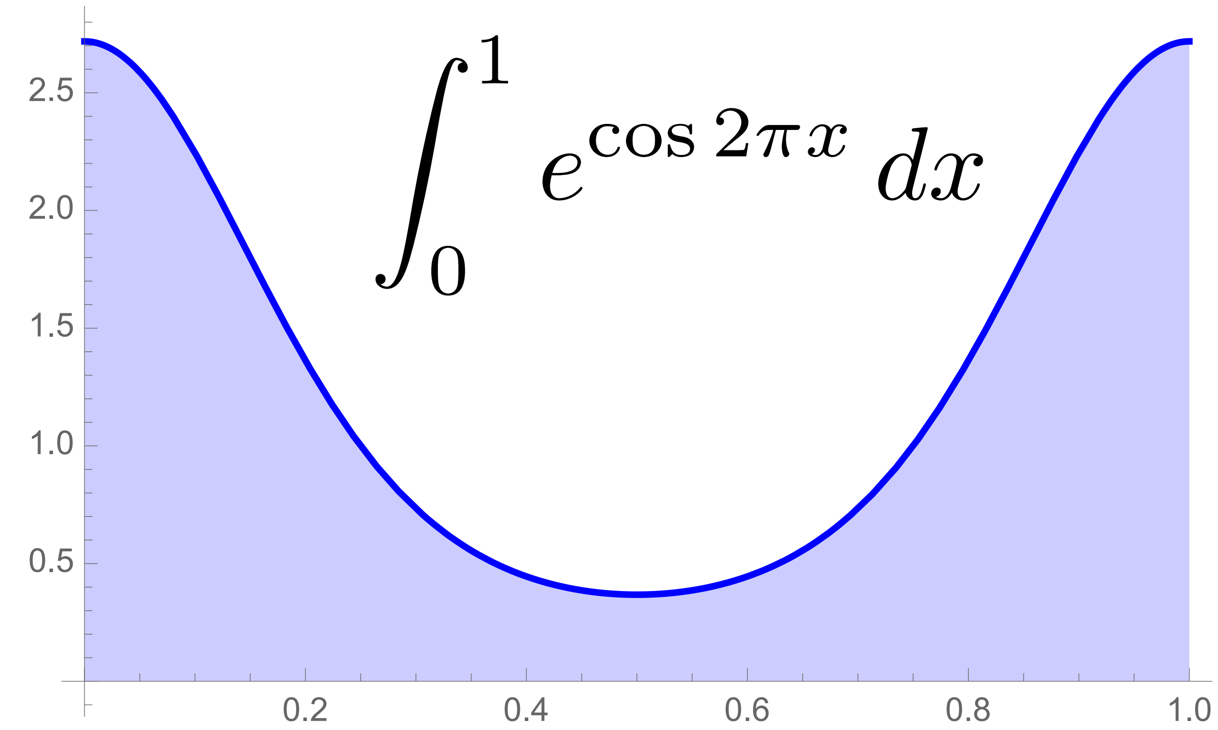

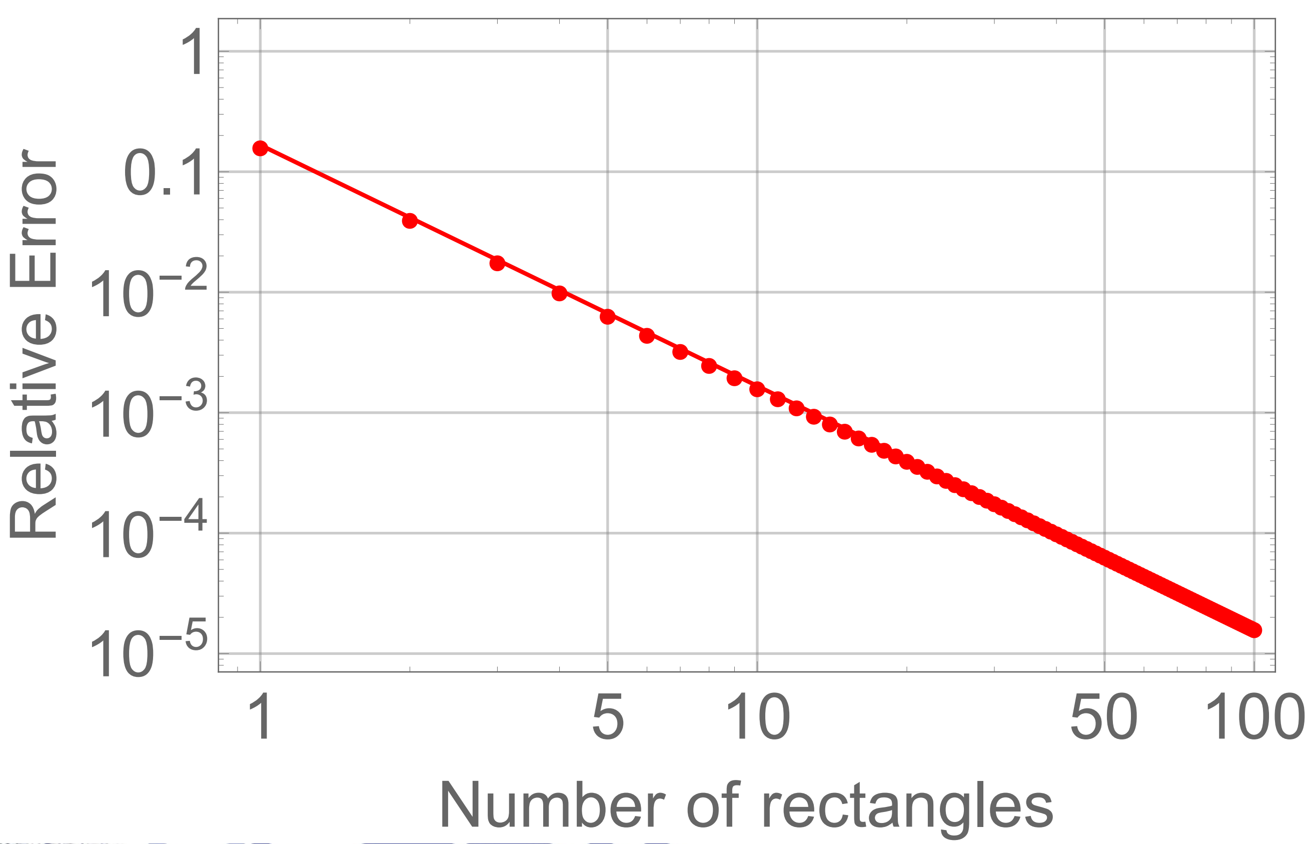

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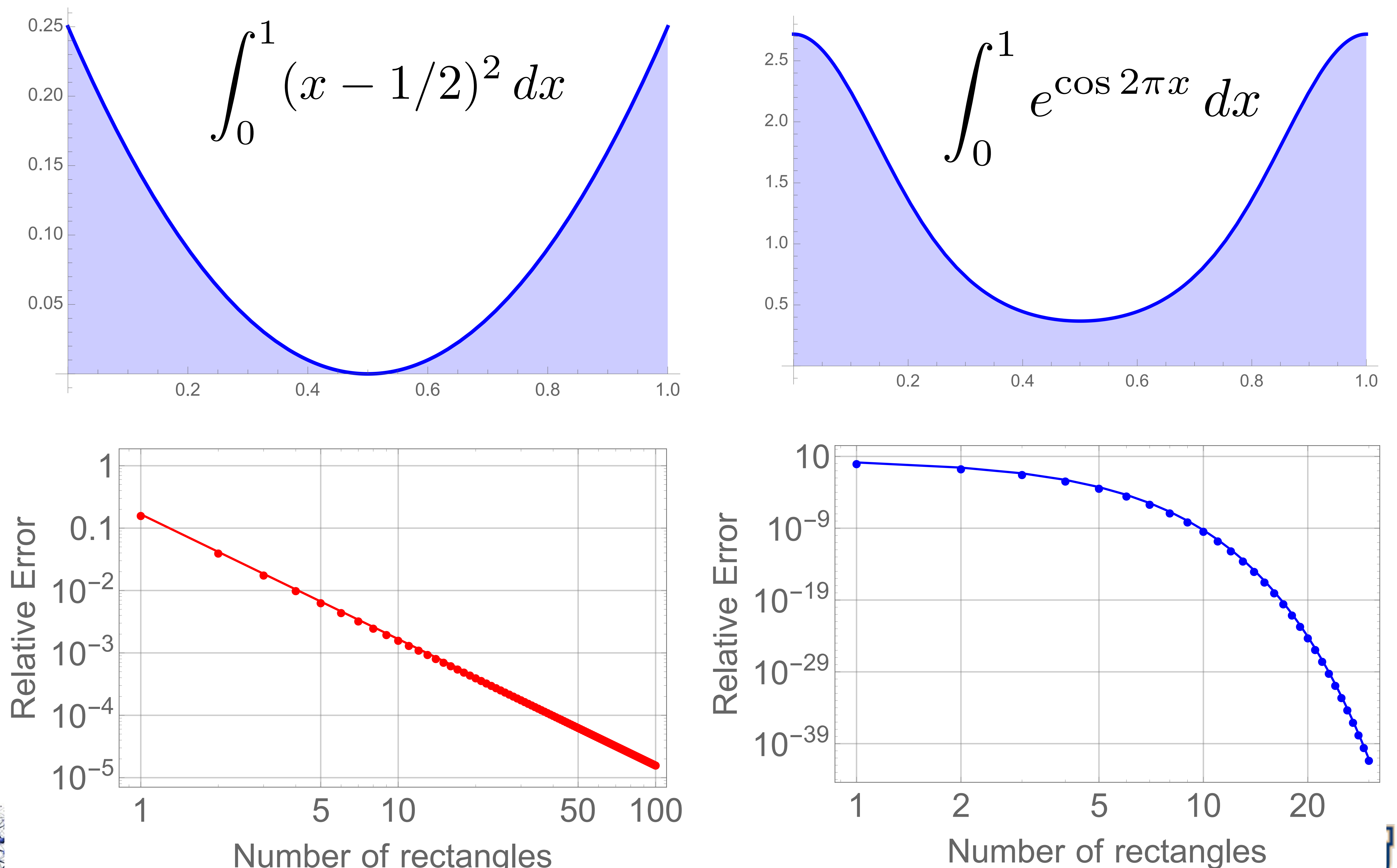

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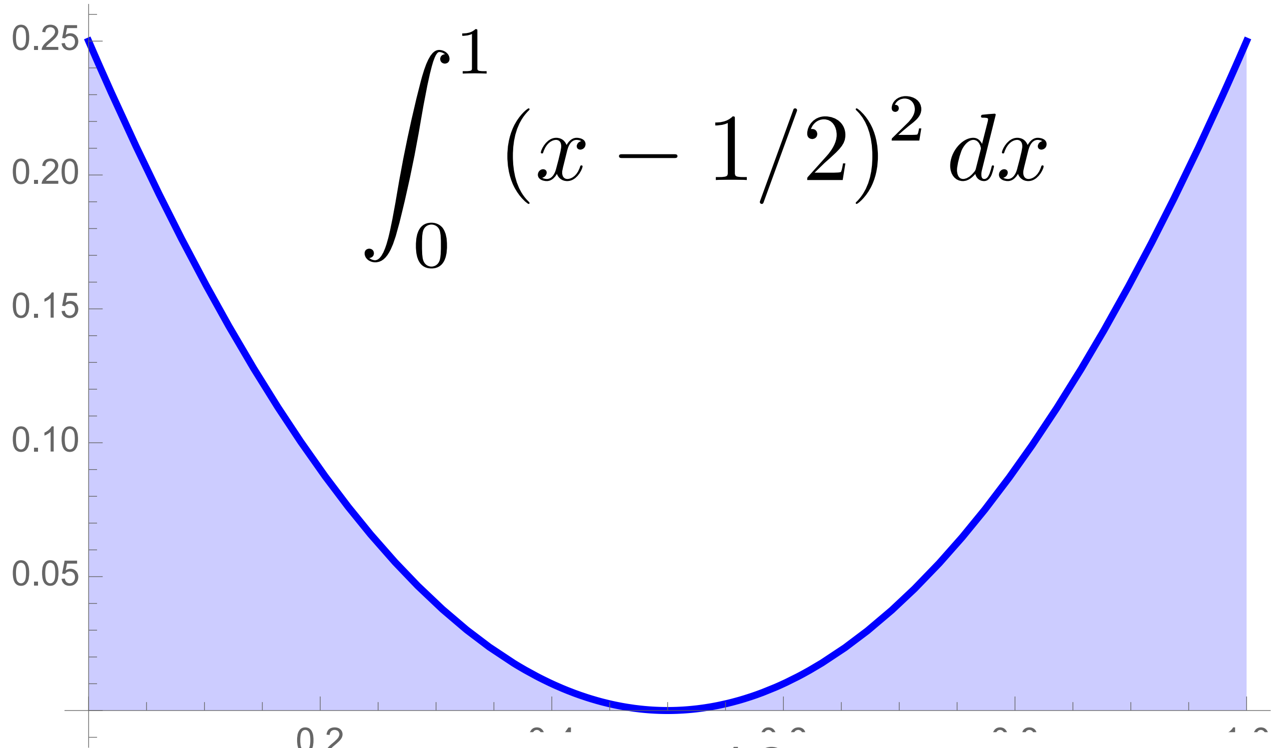

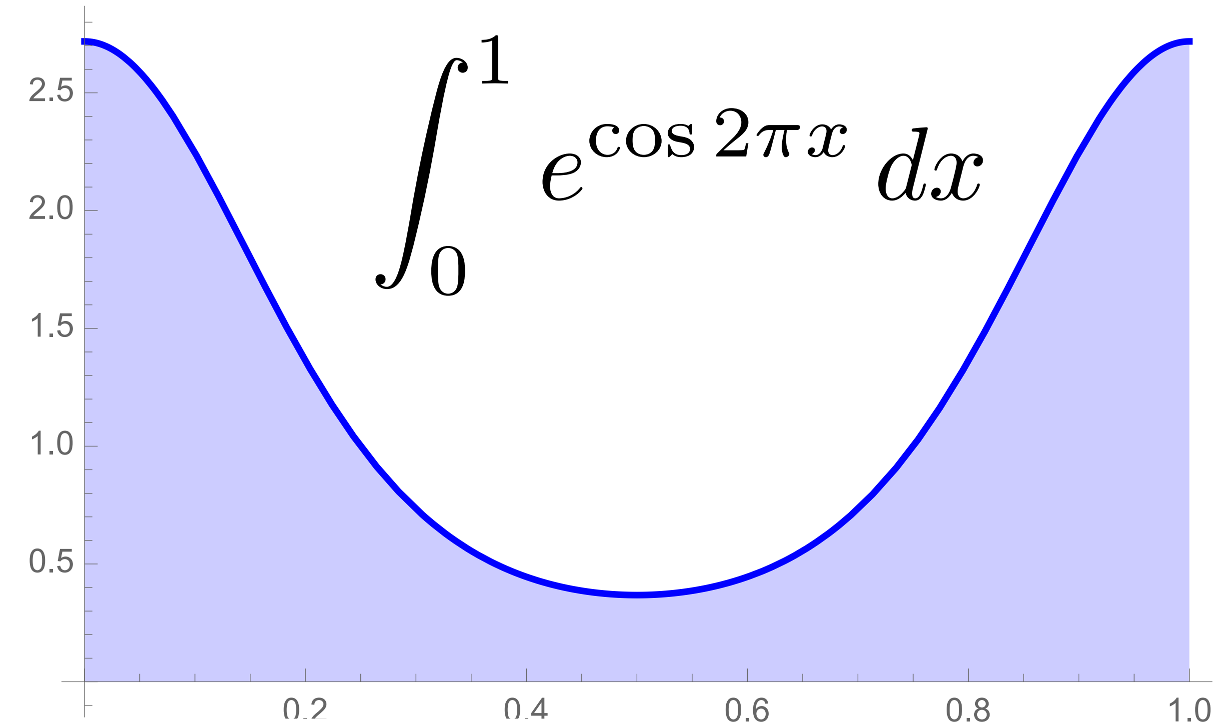

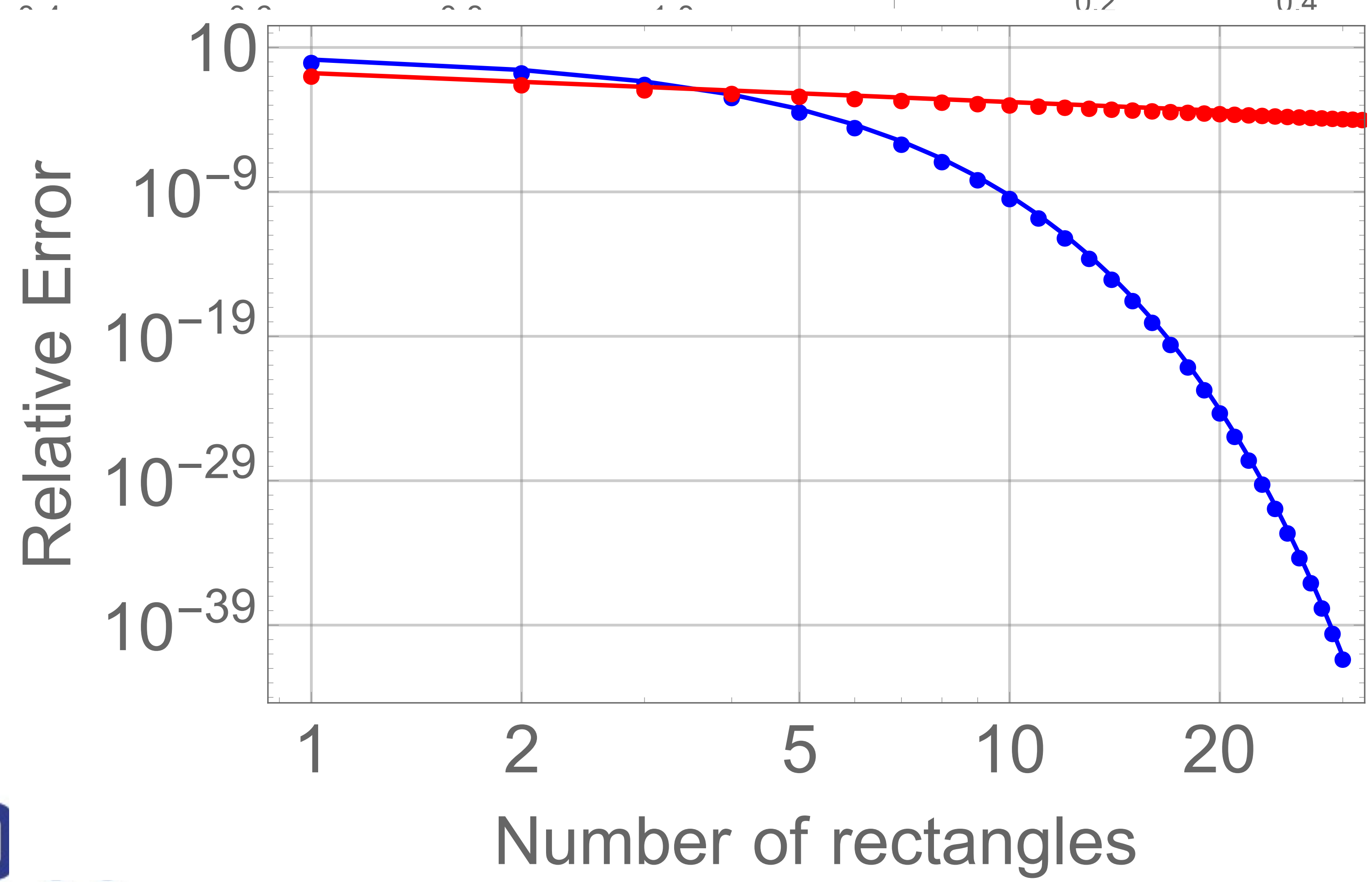

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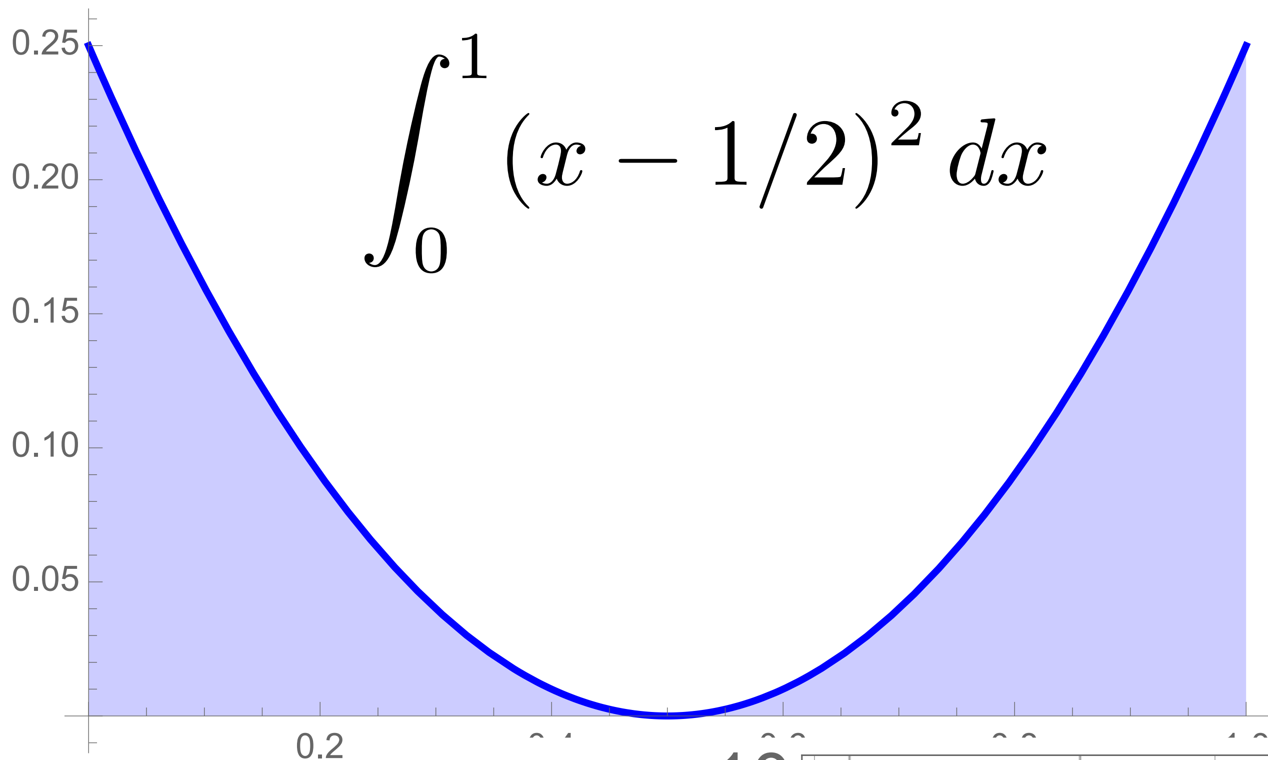

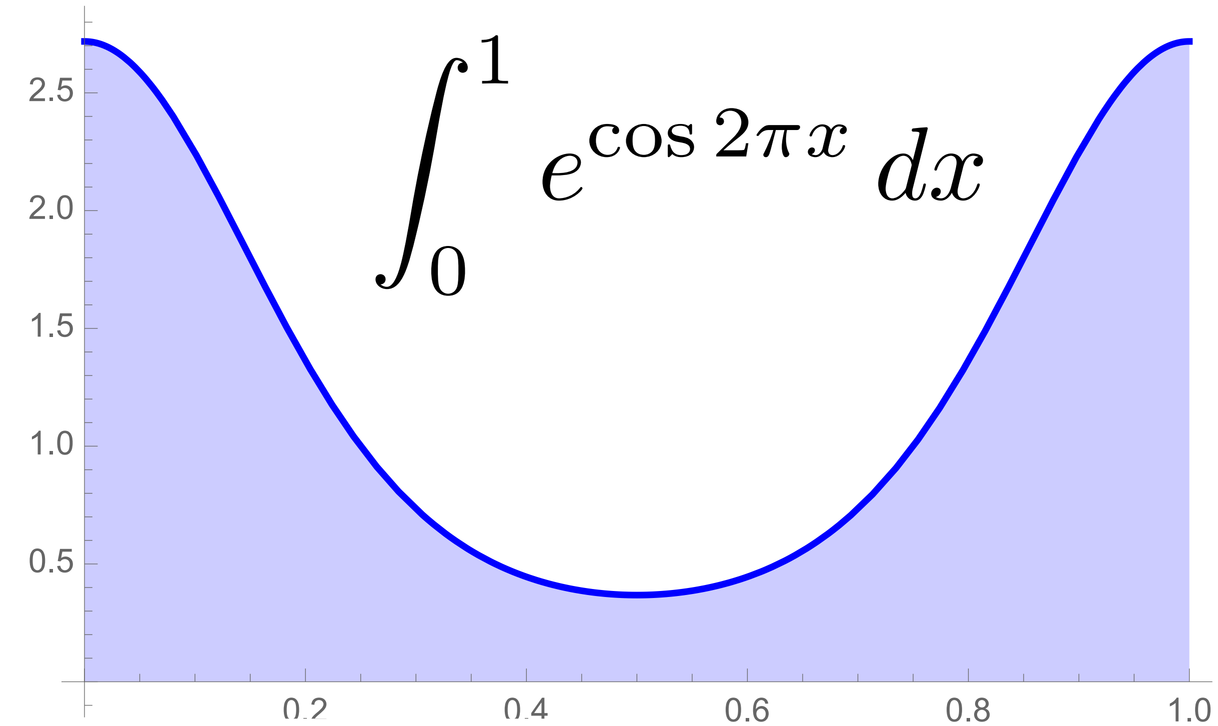

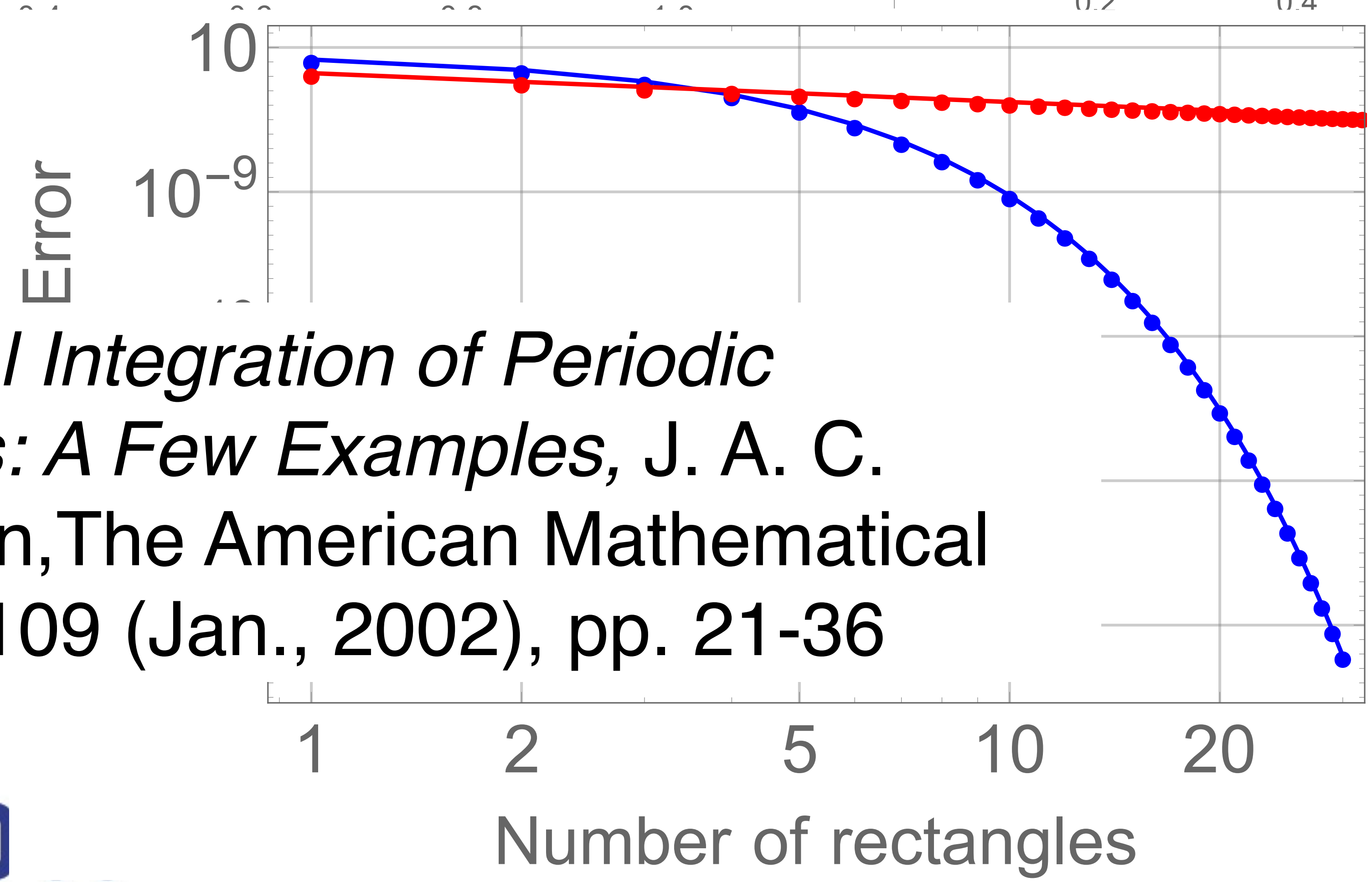

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Special points for Brillouin-zone integrations*

Hendrik J. Monkhorst and James D. Pack
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(Received 21 January 1976)

A method is given for generating sets of special points in the Brillouin zone which provides an efficient means of integrating periodic functions of the wave vector. The integration can be over the entire Brillouin zone or over specified portions thereof. This method also has applications in spectral and density-of-state calculations. The relationships to the Chadi-Cohen and Gilat-Raubenheimer methods are indicated.

I. INTRODUCTION

Many calculations in crystals involve integrating

$$\vec{b}_1 = \frac{2\pi}{v}\vec{t}_2\times\vec{t}_3\,,\quad \vec{b}_2 = \frac{2\pi}{v}\vec{t}_3\times\vec{t}_1\,,\quad \vec{b}_3 = \frac{2\pi}{v}\vec{t}_1\times\vec{t}_2\,.$$

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