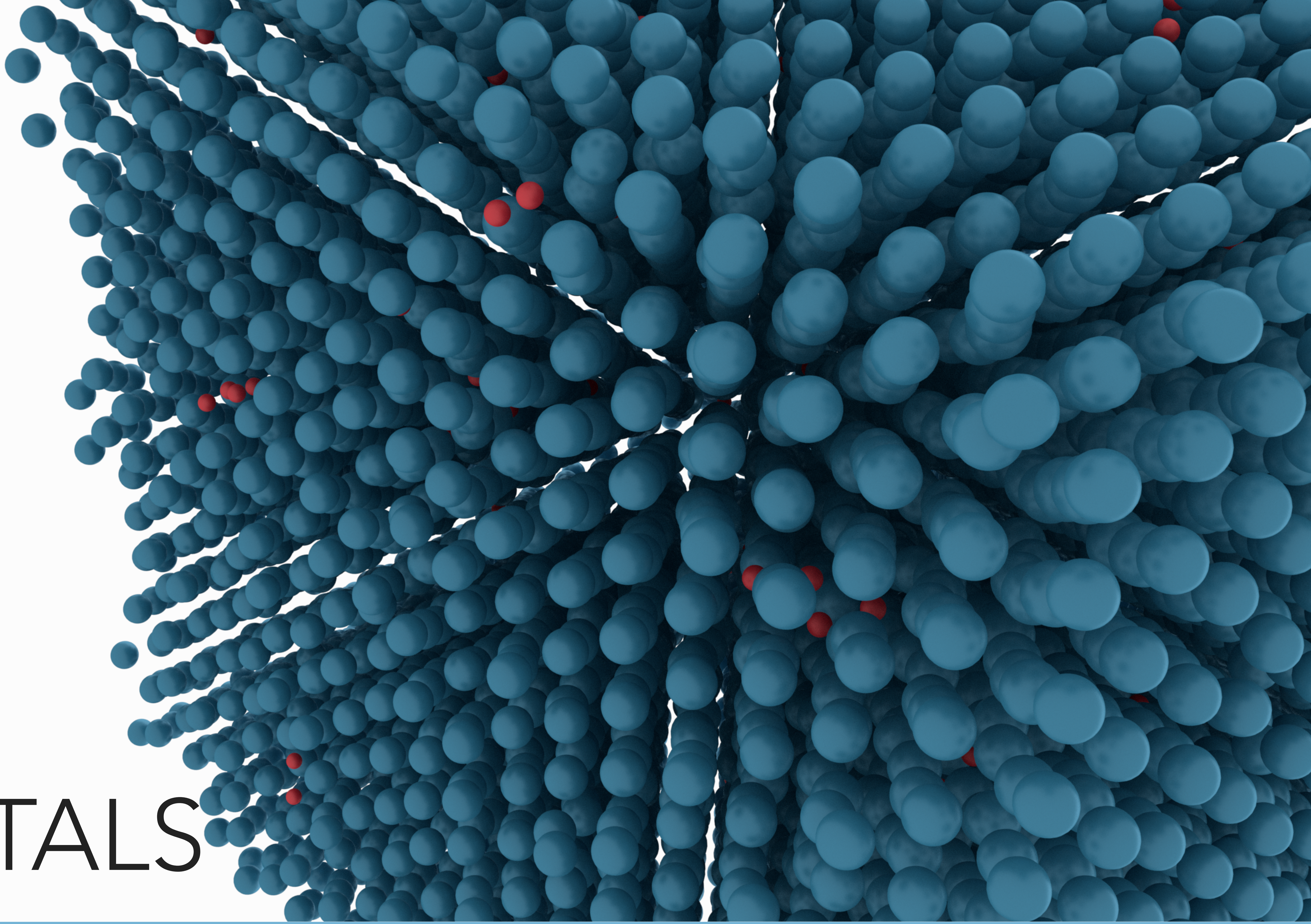
ANOMALOUS DYNAMICS AND PHASE BEHAVIOUR OF DOPANTS IN WEAK CRYSTALS



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100years 1918 — 2018

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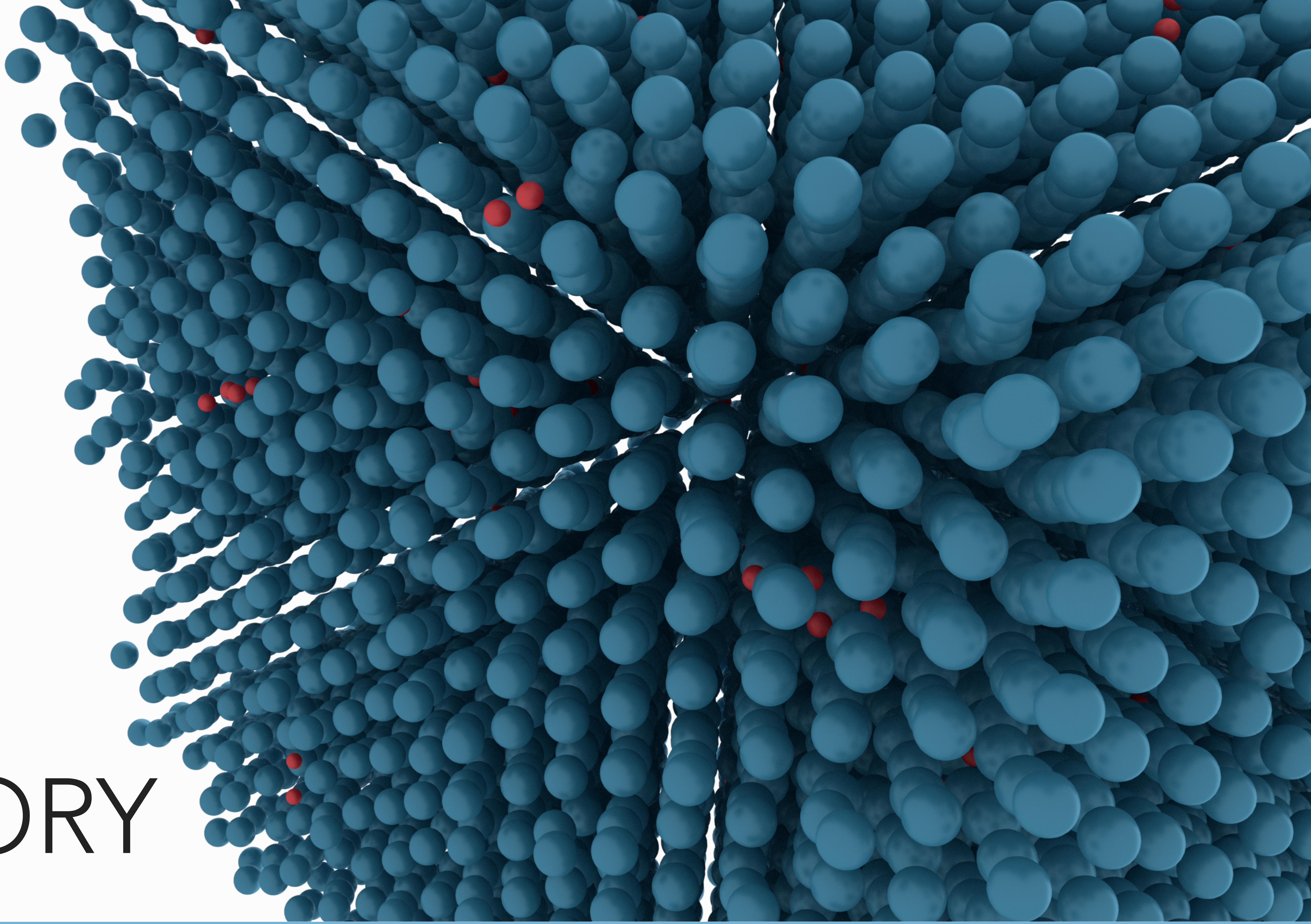
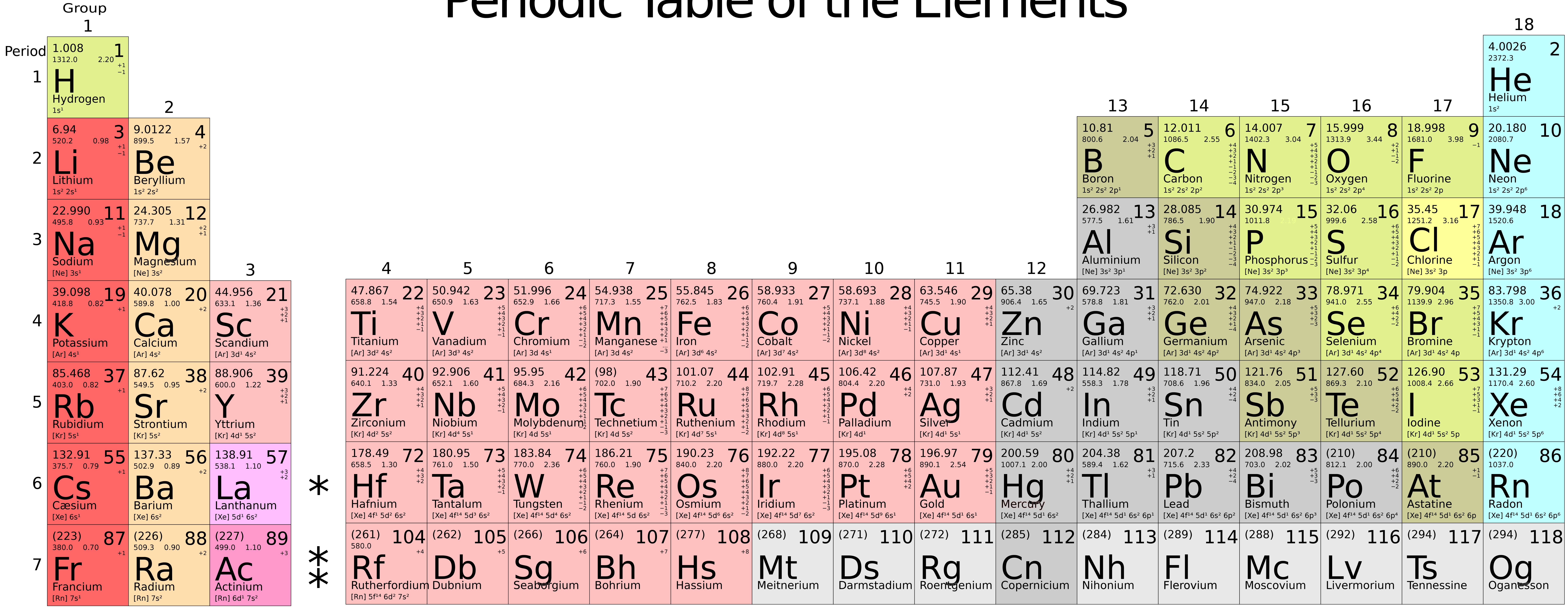
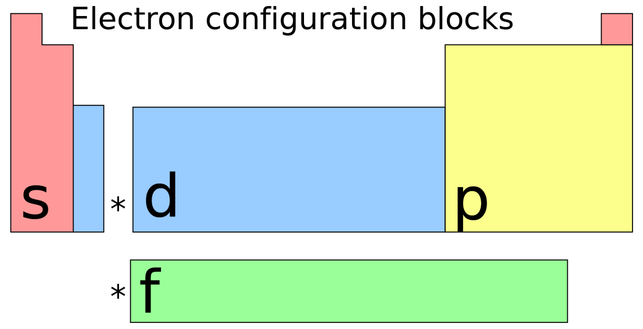
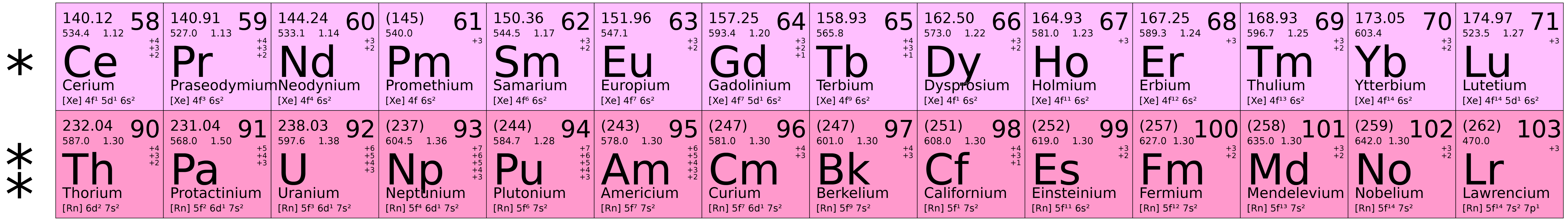
ENTROPIC CRYSTALS AND THE FAILURE OF LATTICE THEORY



Periodic Table of the Elements







Notes

- 1 kJ/mol ≈ 96.485 eV
- all elements are implied to have an oxidation state of zero.

by Robert Campion / updated 2016, 2018

alkali metals · alkaline earth metals · lanthanides · actinides · transition metals · unknown properties · post-transition metals · metalloids · reactive nonmetals · noble gases

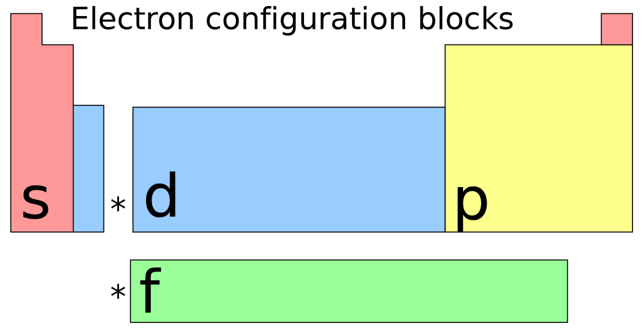
Periodic Table of the Elements

Group 1 … 18; Period 1 … 7

3	Li	Lithium	6.94	520.2	0.98	+1, −1	$1s^2 2s^1$	Group 1	Period 2
11	Na	Sodium	22.990	495.8	0.93	+1, −1	$[Ne]\ 3s^1$	Group 1	Period 3
19	K	Potassium	39.098	418.8	0.82	+1	$[Ar]\ 4s^1$	Group 1	Period 4
37	Rb	Rubidium	85.468	403.0	0.82	+1	$[Kr]\ 5s^1$	Group 1	Period 5
55	Cs	Cæsium	132.91	375.7	0.79	+1	$[Xe]\ 6s^1$	Group 1	Period 6
87	Fr	Francium	(223)	380.0	0.70	+1	$[Rn]\ 7s^1$	Group 1	Period 7
56	Ba	Barium	137.33	502.9	0.89	+2	$[Xe]\ 6s^2$	Group 2	Period 6
88	Ra	Radium	(226)	509.3	0.90	+2	$[Rn]\ 7s^2$	Group 2	Period 7
23	V	Vanadium	50.942	650.9	1.63	+5, +4, +3, +2, +1, −1	$[Ar]\ 3d^3 4s^2$	Group 5	Period 4
41	Nb	Niobium	92.906	652.1	1.60	+5, +4, +3, +2, −1	$[Kr]\ 4d^4 5s^1$	Group 5	Period 5
73	Ta	Tantalum	180.95	761.0	1.50	+5, +4, +3, +2, −1	$[Xe]\ 4f^{14} 5d^3 6s^2$	Group 5	Period 6
105	Db	Dubnium	(262)			+5		Group 5	Period 7
24	Cr	Chromium	51.996	652.9	1.66	+6, +5, +4, +3, +2, +1, −1, −2	$[Ar]\ 3d\ 4s^1$	Group 6	Period 4
42	Mo	Molybdenum	95.95	684.3	2.16	+6, +5, +4, +3, +2, +1, −1, −2	$[Kr]\ 4d\ 5s^1$	Group 6	Period 5
74	W	Tungsten	183.84	770.0	2.36	+6, +5, +4, +3, +2, +1, −1, −2	$[Xe]\ 4f^{14} 5d^4 6s^2$	Group 6	Period 6
106	Sg	Seaborgium	(266)			+6		Group 6	Period 7
25	Mn	Manganese	54.938	717.3	1.55	+7, +6, +5, +4, +3, +2, +1, …, −3	$[Ar]\ 3d\ 4s^2$	Group 7	Period 4
26	Fe	Iron	55.845	762.5	1.83	+6, +5, +4, +3, +2, +1, −1, −2	$[Ar]\ 3d^6 4s^2$	Group 8	Period 4
110	Ds	Darmstadium	(271)					Group 10	Period 7
111	Rg	Roentgenium	(272)					Group 11	Period 7
112	Cn	Copernicium	(285)					Group 12	Period 7
63	Eu	Europium	151.96	547.1		+3, +2	$[Xe]\ 4f^7 6s^2$	*	

Groups: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18

Electron configuration blocks



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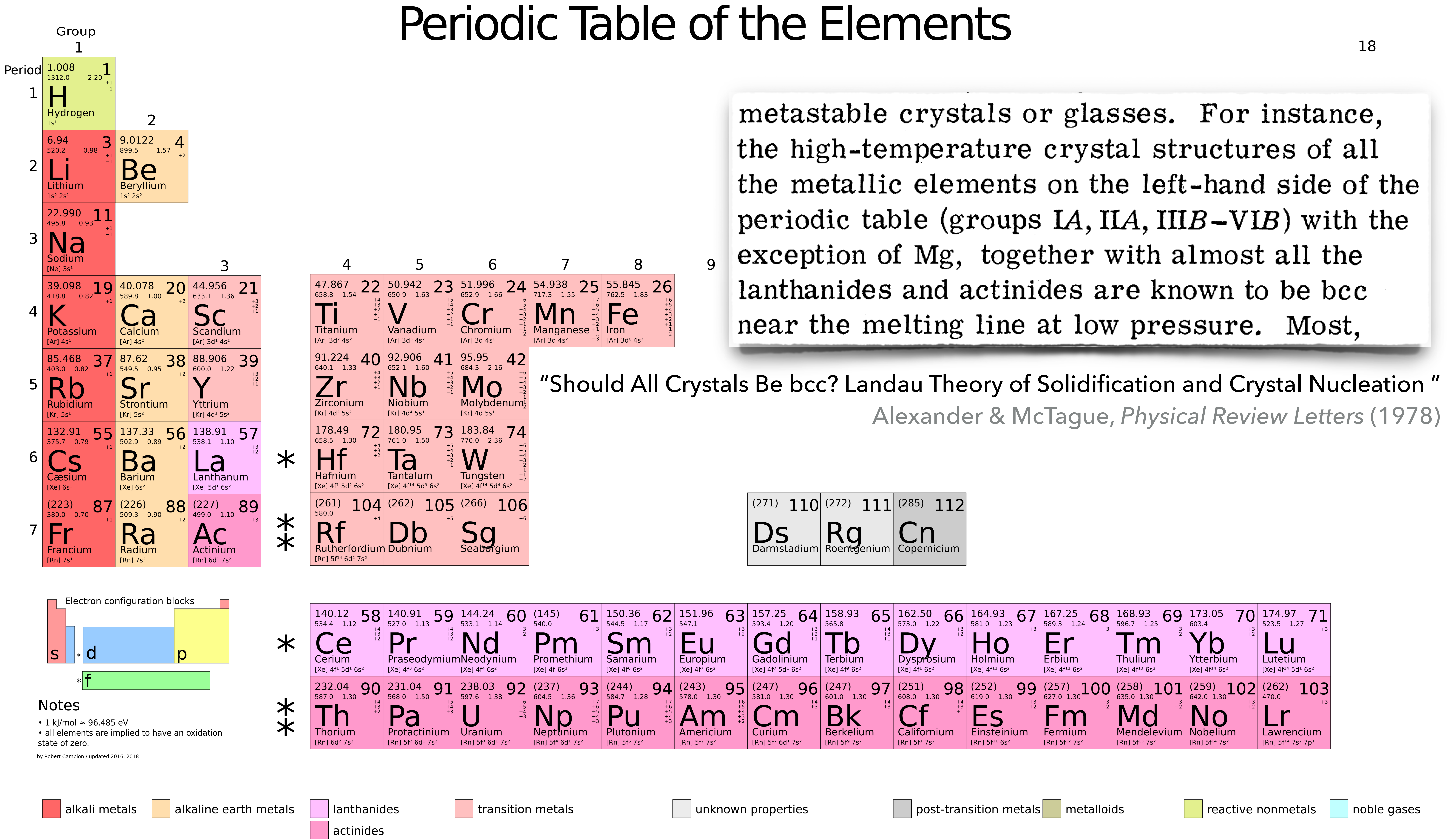


metastable crystals or glasses. For instance, the high-temperature crystal structures of all the metallic elements on the left-hand side of the periodic table (groups IA, IIA, III*B*–VI*B*) with the exception of Mg, together with almost all the lanthanides and actinides are known to be bcc near the melting line at low pressure. Most,

"Should All Crystals Be bcc? Landau Theory of Solidification and Crystal Nucleation "

Alexander & McTague, *Physical Review Letters* (1978) in Hf, Zr and Ti. *The bcc structure in these elements is stabilized at high temperatures only by the entropy contribution.* The same applies for δ-Fe, Na, Li (and for many bcc alloys). We shall now examine the reasons for

"Physical Metallurgy"

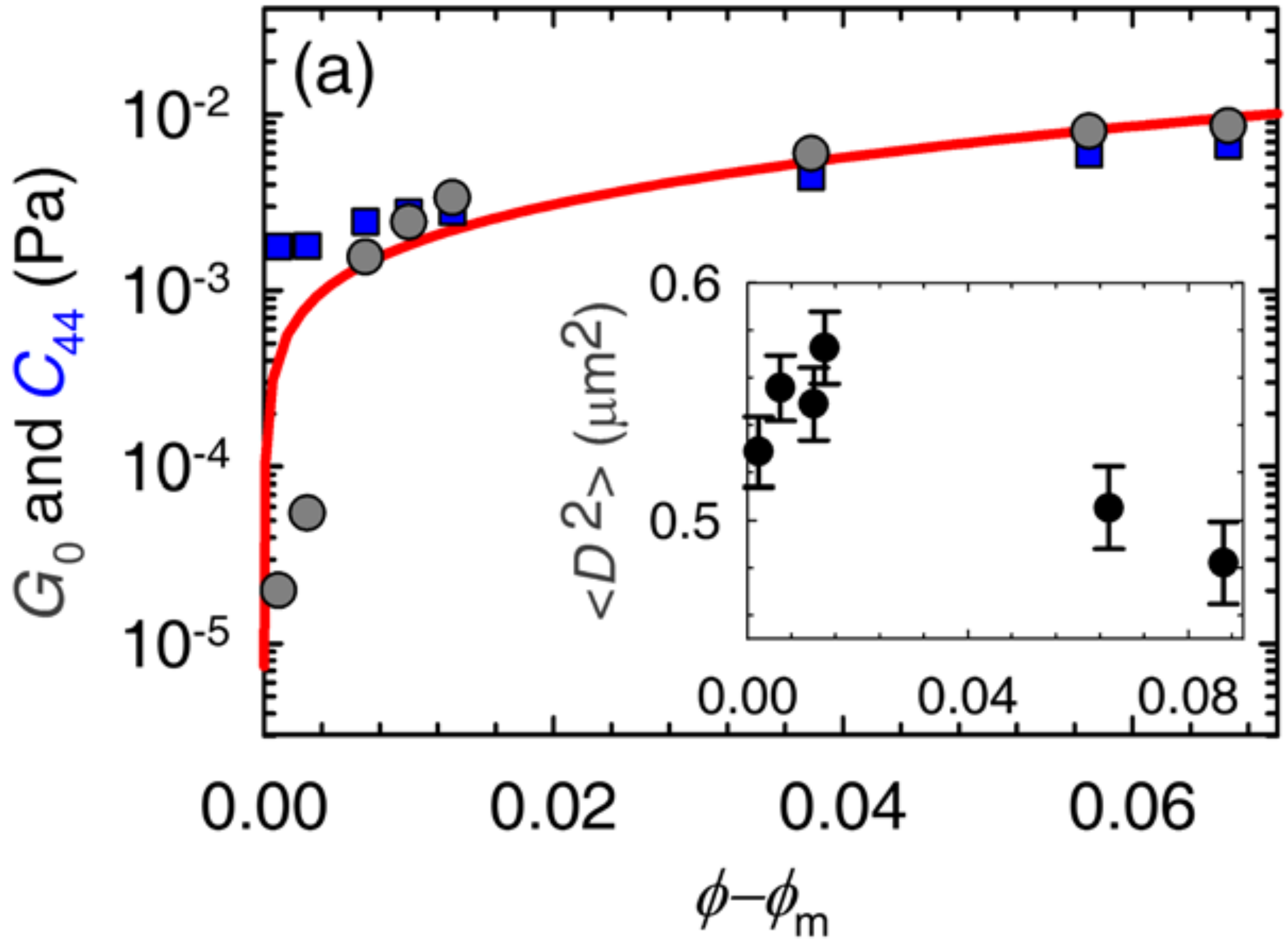
Peter Haasen, *Third Edition* (1996)

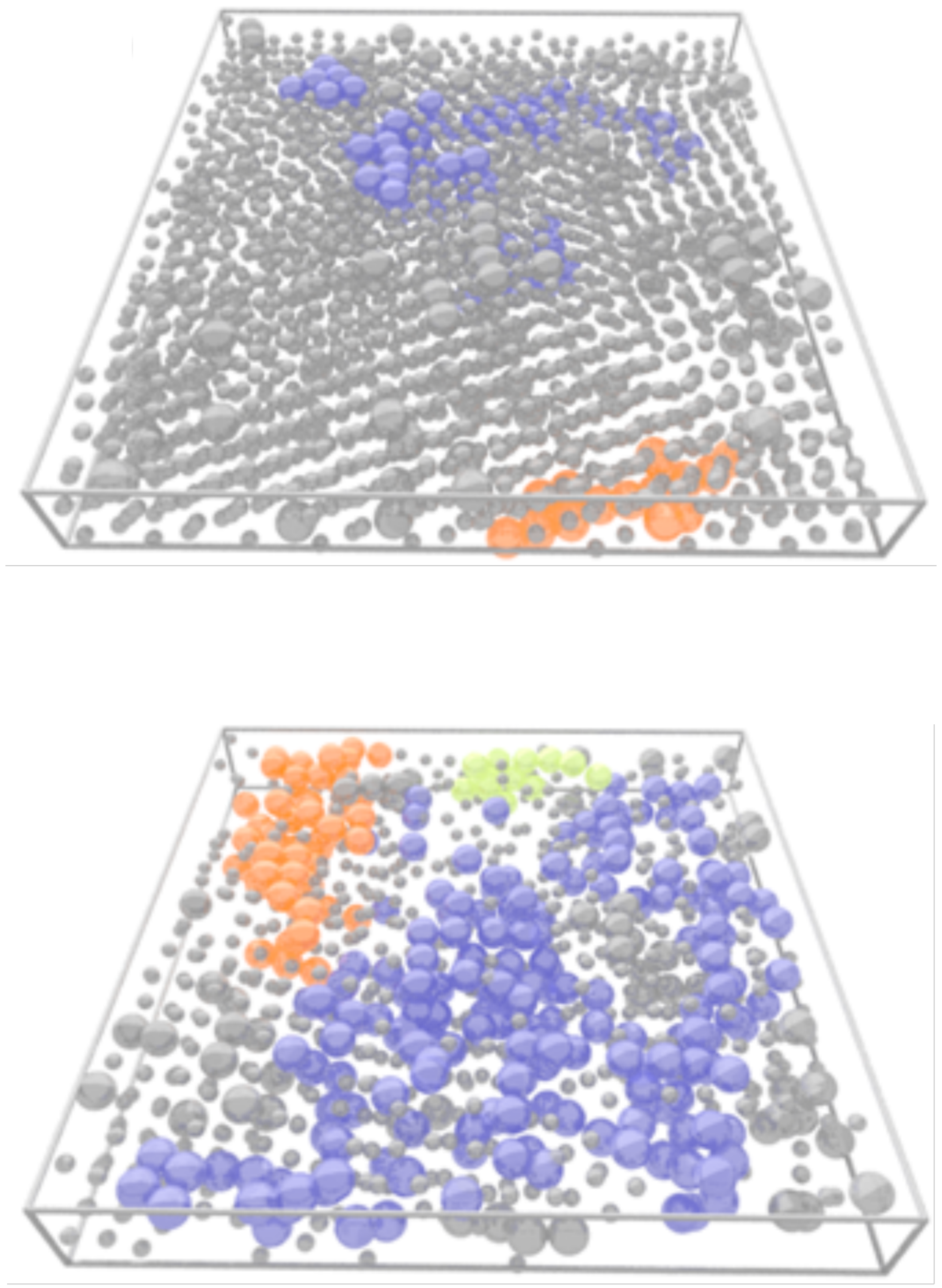
curs with great ease. There is thus strong evidence that bcc is favored by a universal factor.

sion that bcc should be favored near the melting line when the first-order character of the transition is not too pronounced. This is presumably

"Should All Crystals Be bcc? Landau Theory of Solidification and Crystal Nucleation"

Alexander & McTague, *Physical Review Letters* (1978)

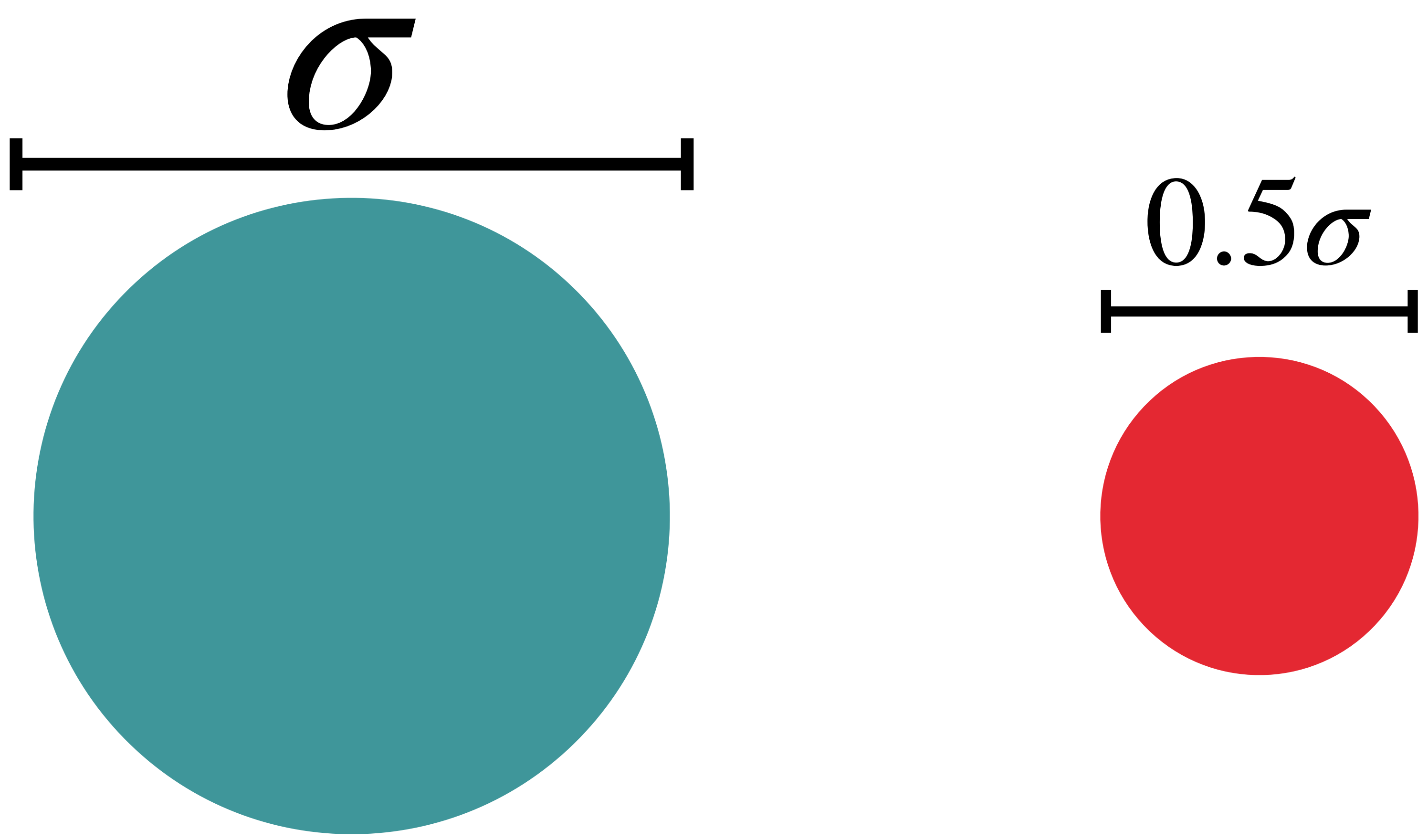




"Direct Observation of Entropic Stabilization of bcc Crystals Near Melting"

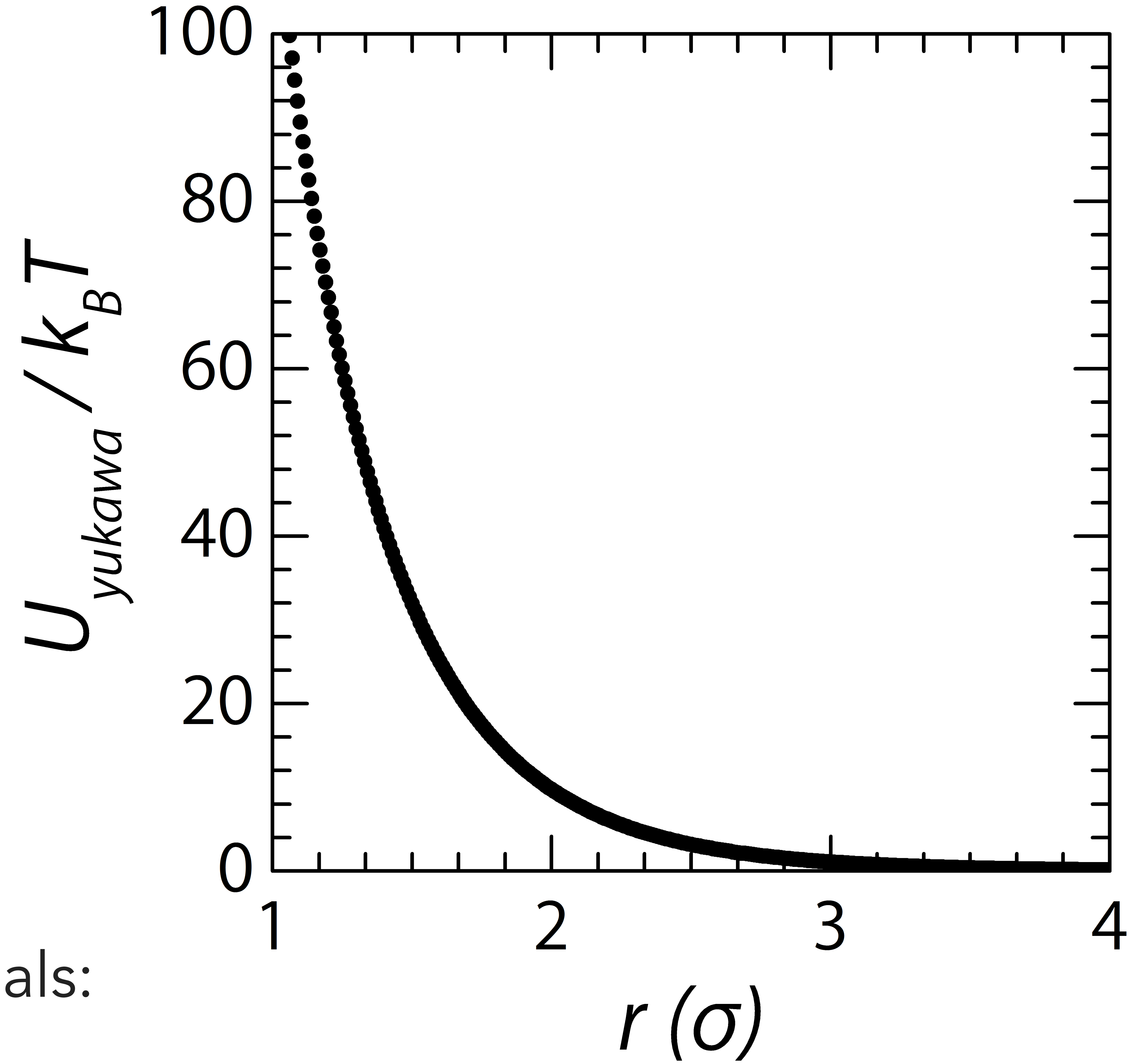
Joris Sprakel, Alessio Zaccone, Frans Spaepen, Peter Schall, and David A. Weitz

Phys. Rev. Lett. **118**, 088003 – Published 23 February 2017

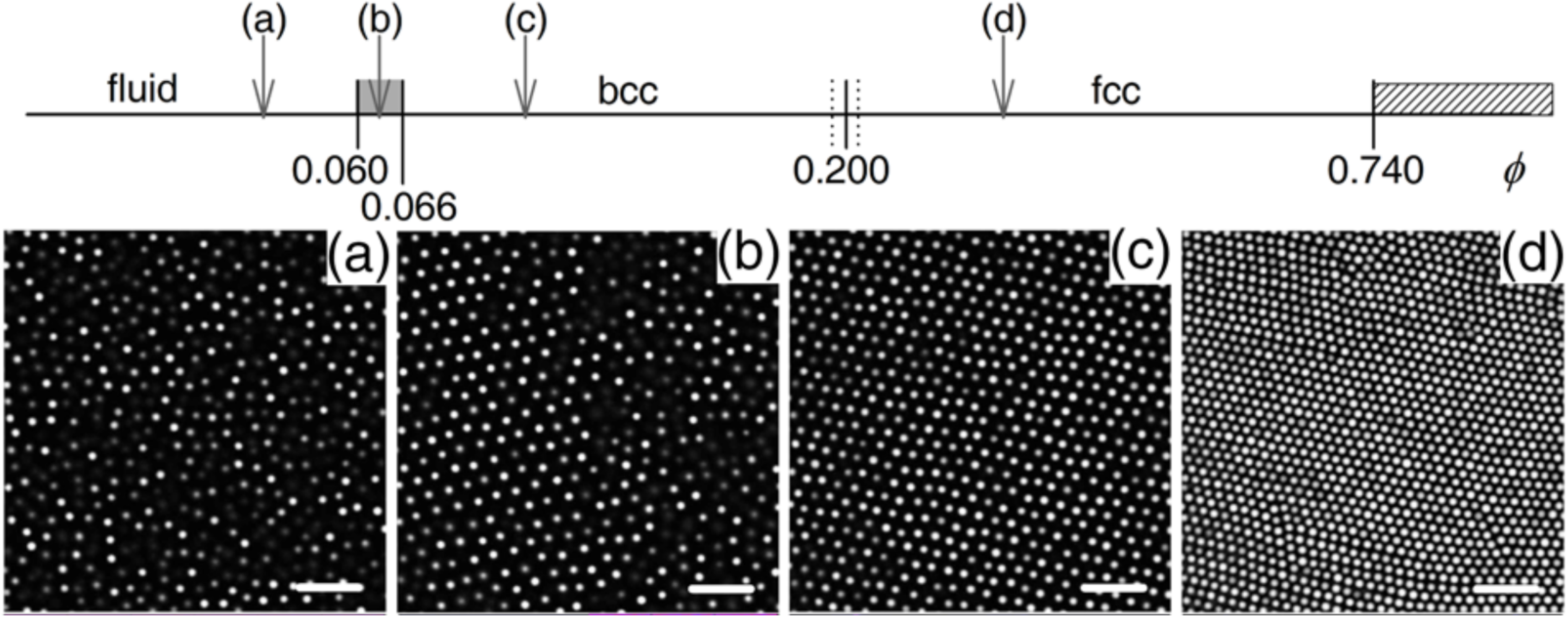


- Brownian Dynamics with HOOMD-Blue
- Interstitial to Base particle ratio: 0.5
- Particles interact with purely repulsive Yukawa potentials:

$$U_{Yukawa}(r) = \varepsilon \frac{\exp\left[-\kappa r\right]}{r}$$



https://bitbucket.org/glotzer/hoomd-blue



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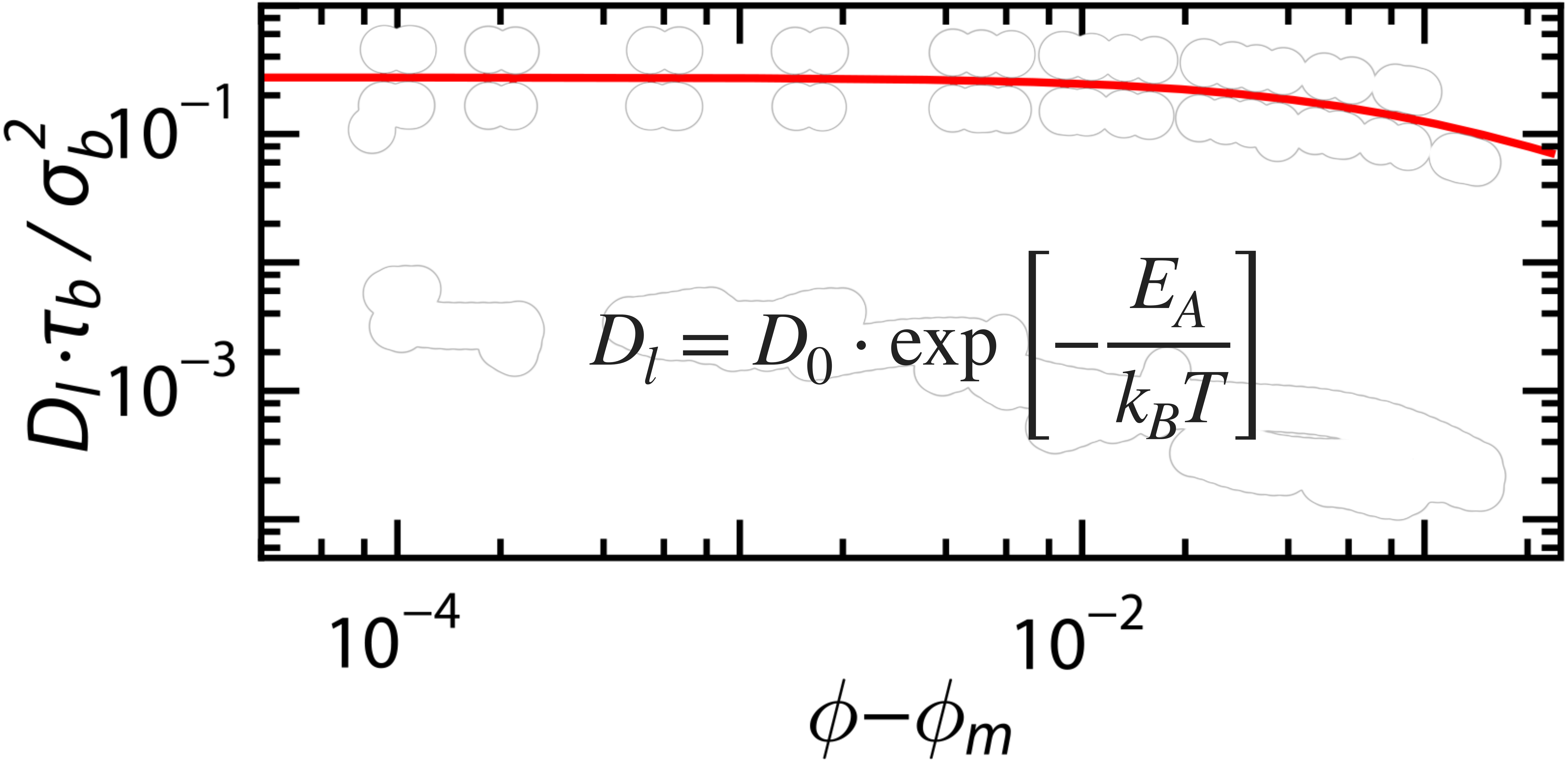
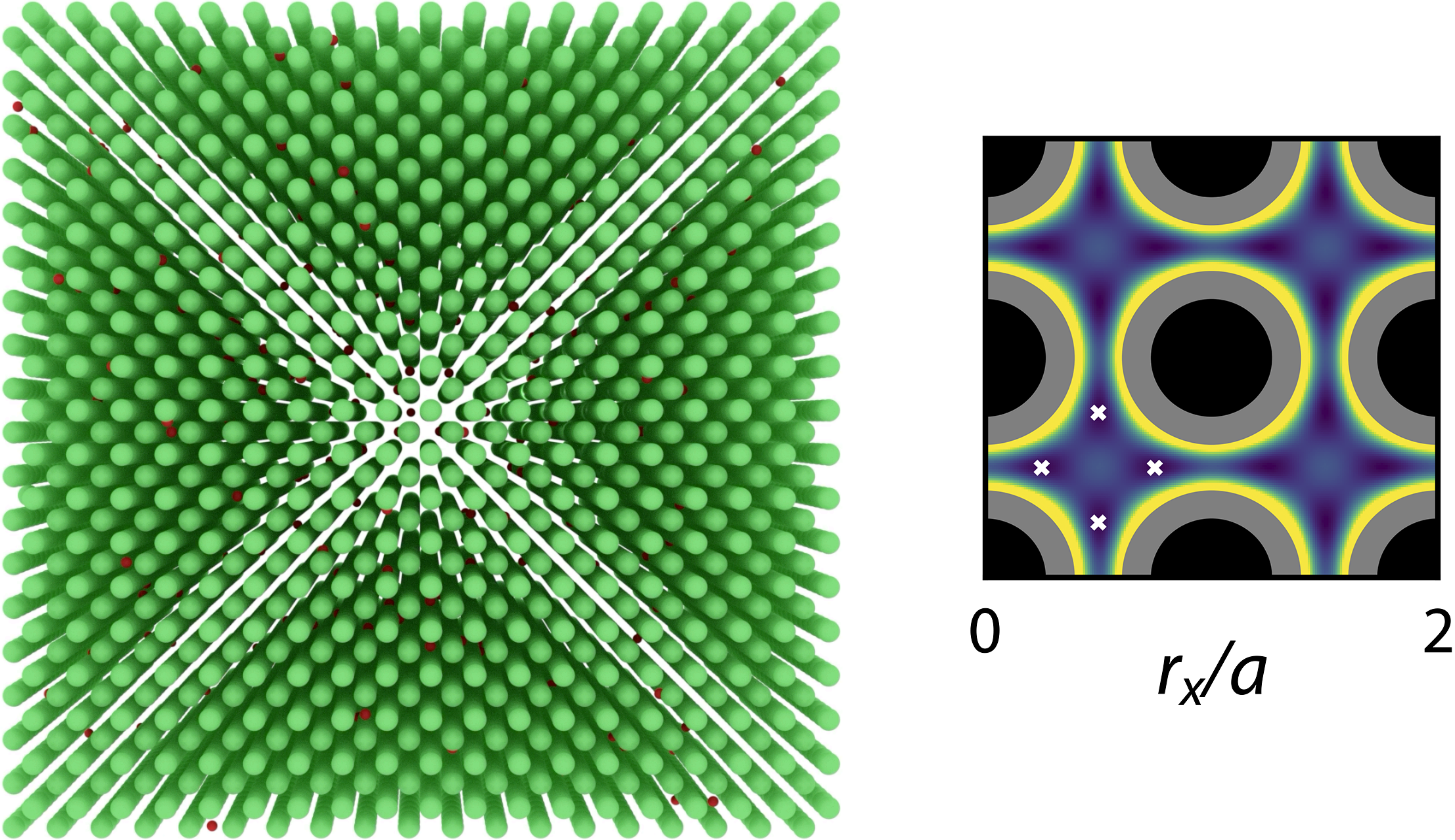
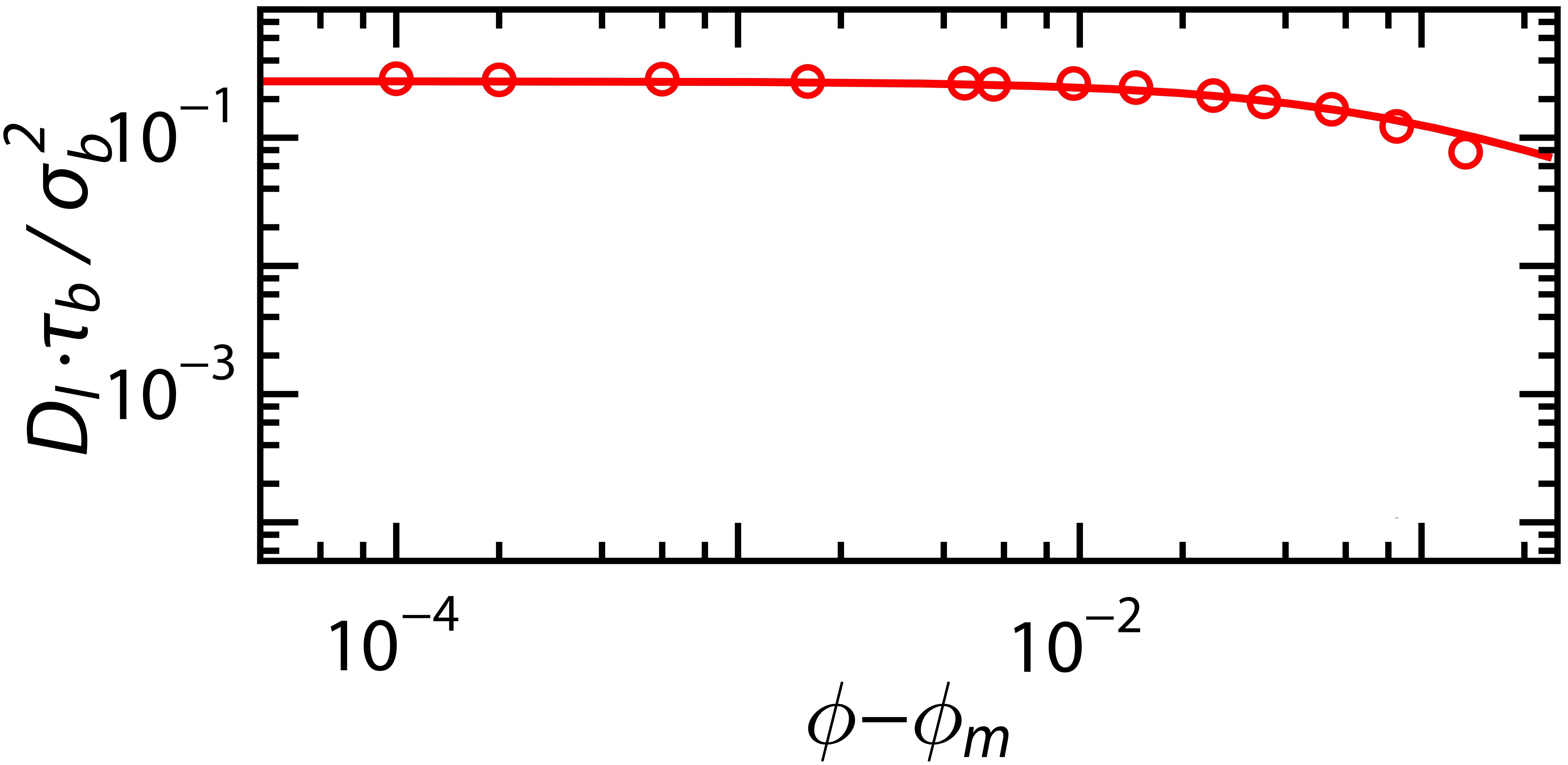


$D_l \cdot \tau_b / \sigma_b^2$
10^{-1}
10^{-3}
$D_l = D_0 \cdot \exp\left[-\frac{E_A}{k_B T}\right]$
10^{-4}
10^{-2}
$\phi - \phi_m$


0
2
r_x/a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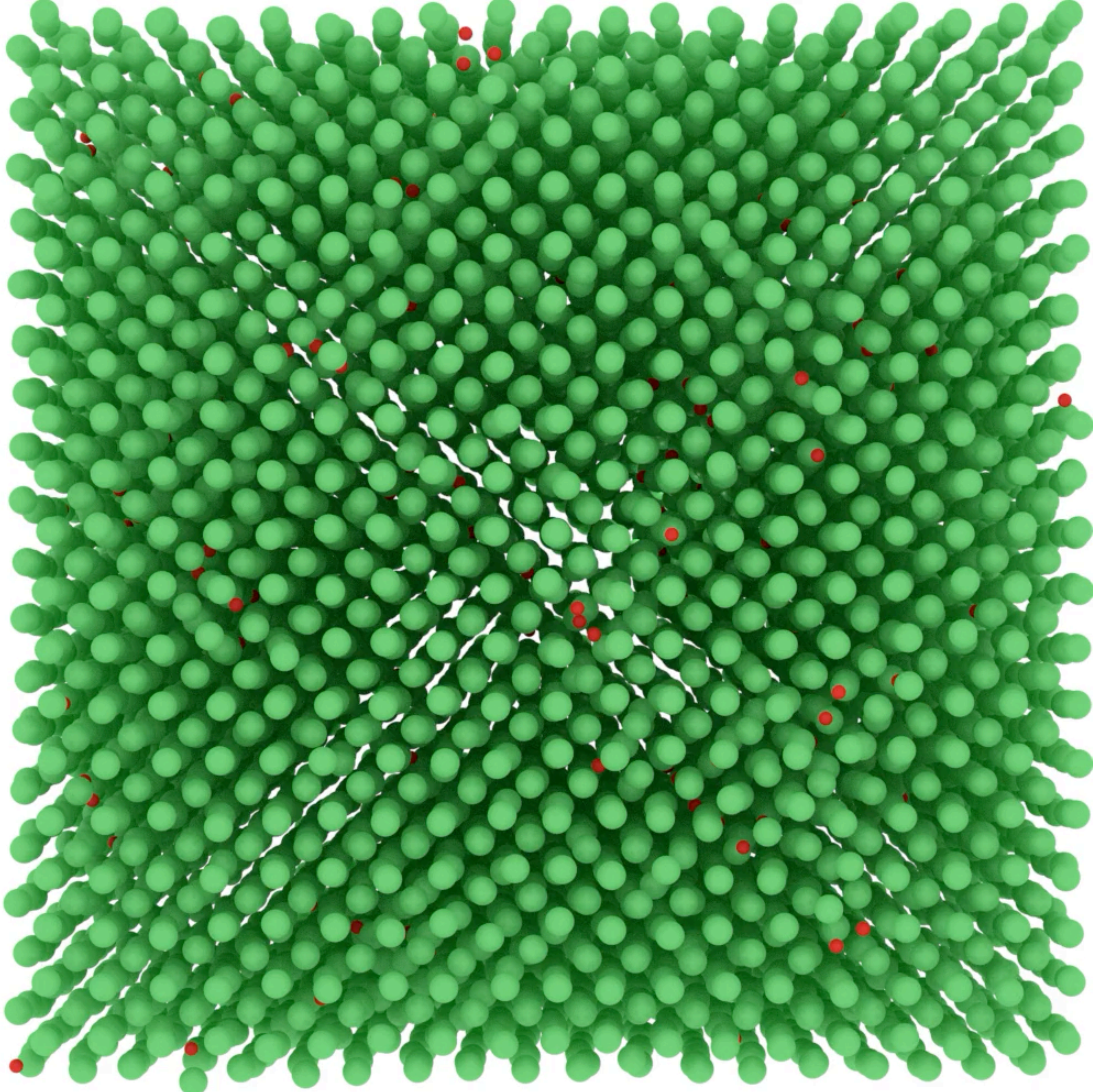

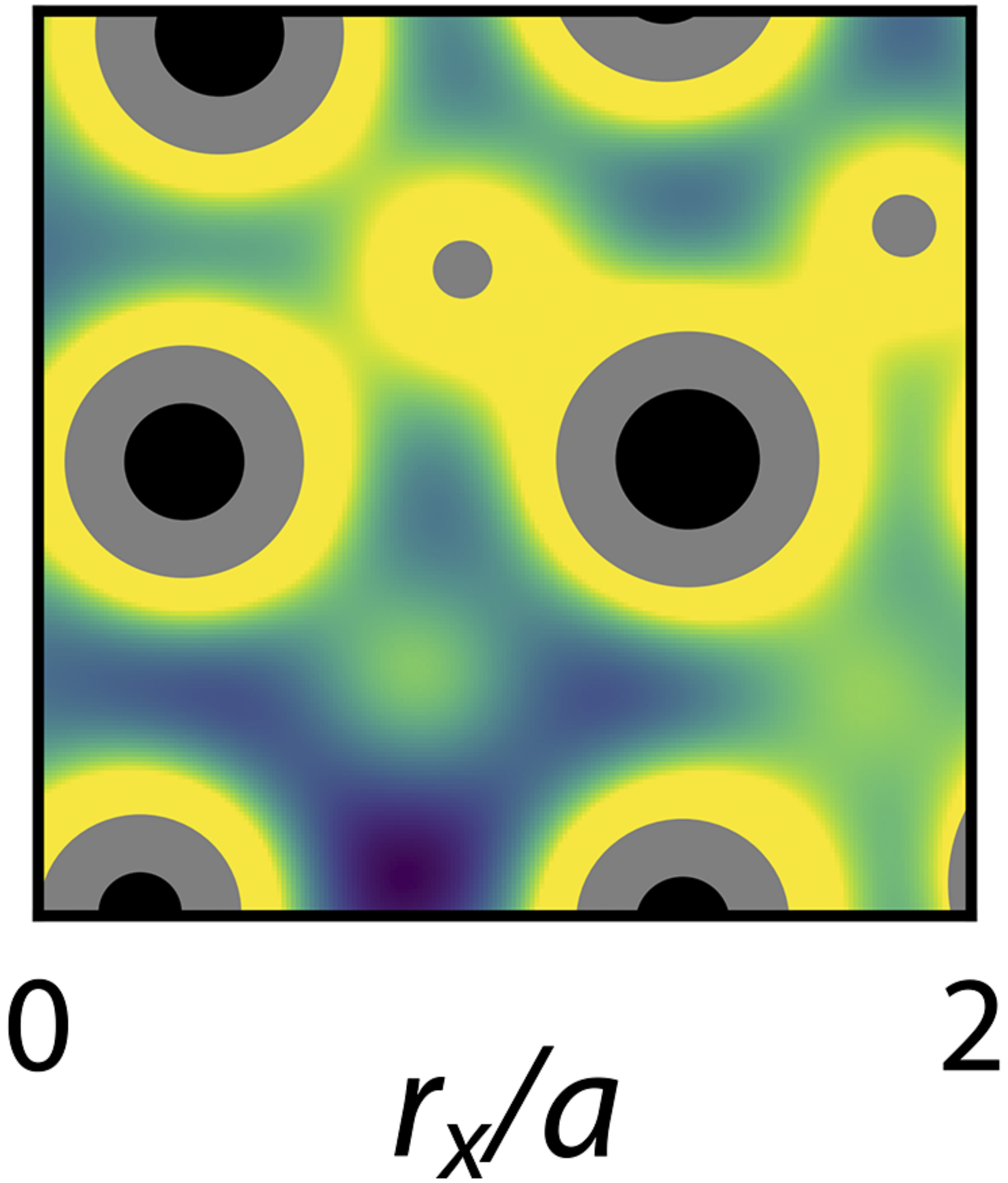
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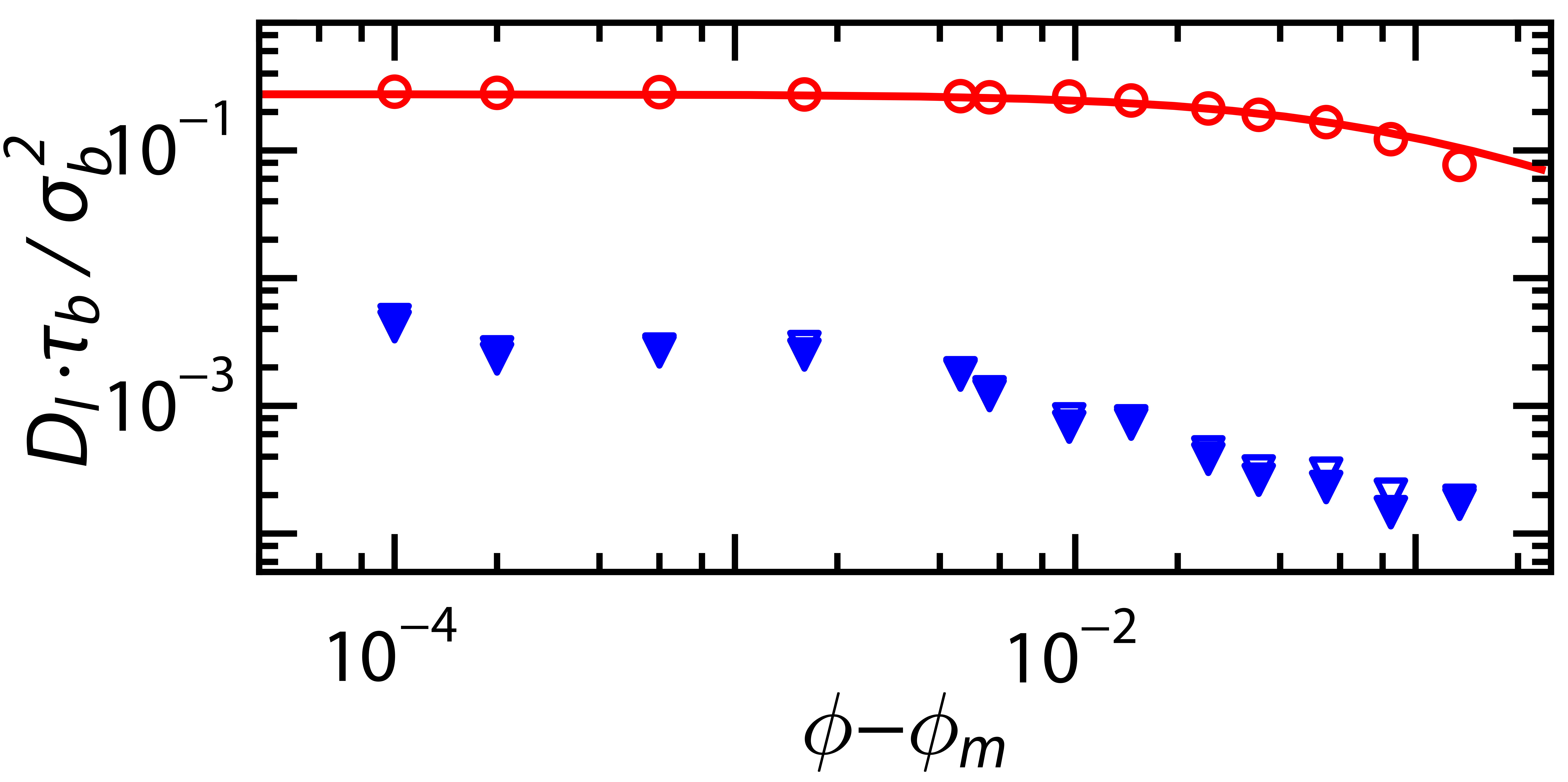

$D_l \cdot \tau_b / \sigma_b^2$
10^{-1}
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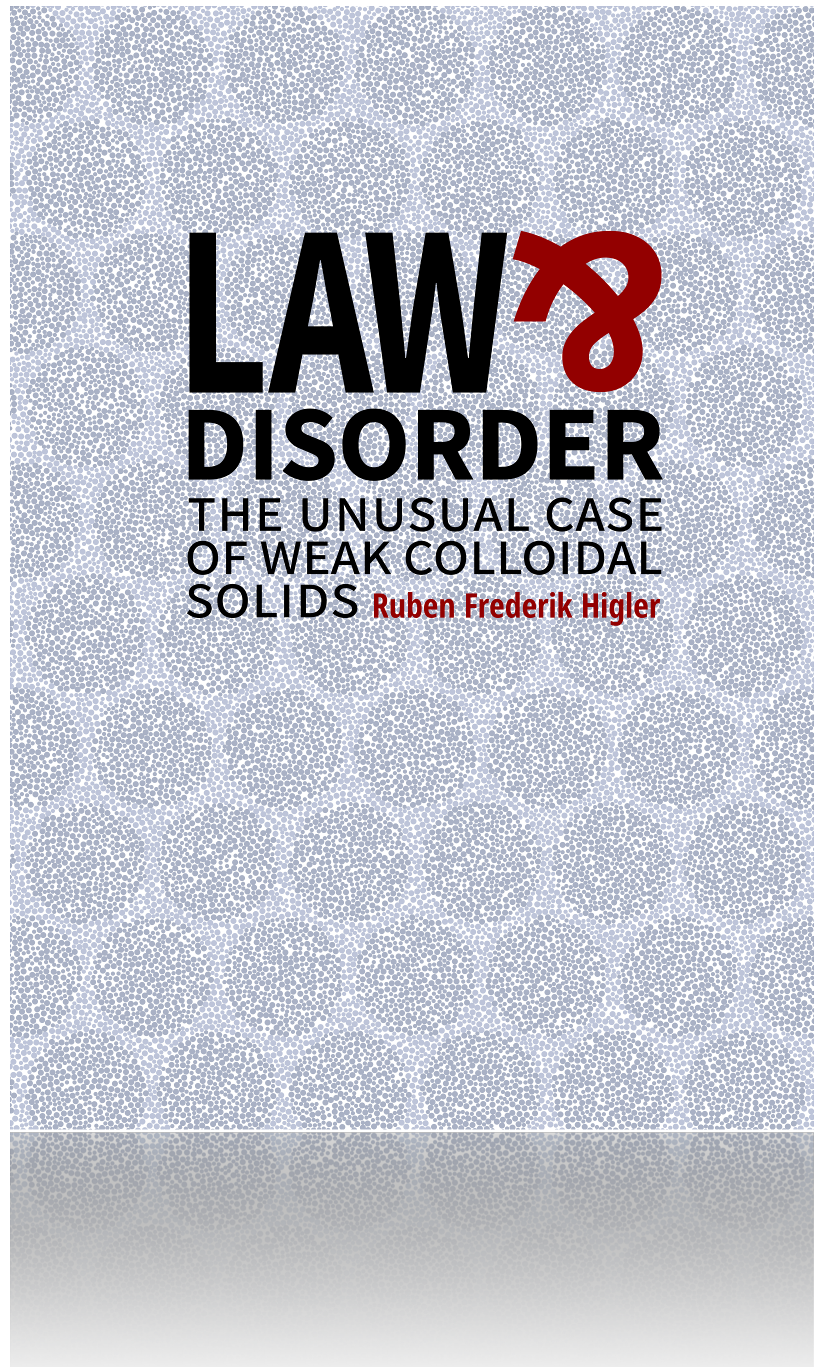
Read More:

"Anomalous dynamics of interstitial dopants in soft crystals "
Justin Tauber*, Ruben Higler* & Joris Sprakel
Proc. Nat. Acad. Sci., **113**, 13660-13665 – Published 29 November 2016

"Doping colloidal bcc crystals – interstitial solids and meta-stable clusters"
Ruben Higler & Joris Sprakel
Scientific Reports, **7**, 12634 – Published 3 October 2017



"Law & disorder – the unusual case of weak colloidal solids"
Ruben Higler
PhD Thesis - 2018