ICYS 2023 DFT Crash Course

Practice on Al metal

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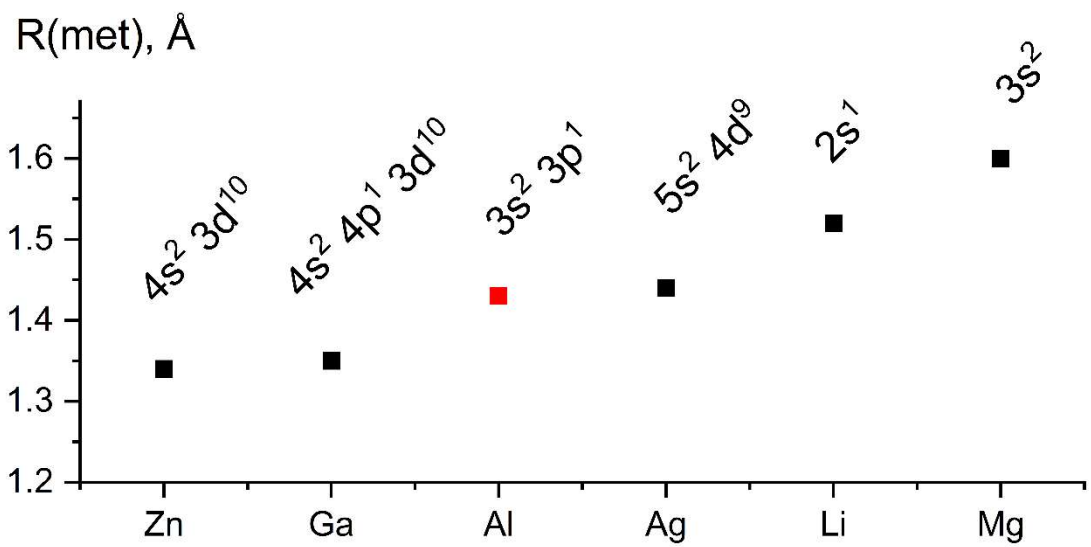
12 ‘friends’ of Al metal

Compositions of solid solutions, at.%:

Zn	65.5	Si	1.5
Ag	23.8	Mn	0.71
Li	16.2	Cr	0.37
Mg	18.9	V	0.2
Ga	5.5	Sc	0.35
Cu	2.5	Ti	0.146

!!!
Maximum compositions up to 500 °C



We take only 6 of them

Mg, Zn – hcp

Al, Ag – ccp

Li – bcc

Ga – distorted hcp (Cmce)

https://extxe.com
https://en.wikipedia.org/wiki/Atomic_radii_of_the_elements_(data_page)

Calculation set

VASP with ‘simanrc’ module

Standart optimization set: (PAW, PBE)

- EDIFF = 1e-05
- NSW = 20
- EDIFFG = -0.025
- IBRION = 1
- ISIF = 3
- ENCUT = 300
- ENAUG = 700.0
- KSPACING = 0.2
- LREAL = Auto
- ISMEAR = 0

Changed on ISIF = 4 for hexagonal Mg and Zn

Changed on ENCUT = 150 for comparison

+

2 supercells for defects:

fcc-cell => 4 atoms per cell

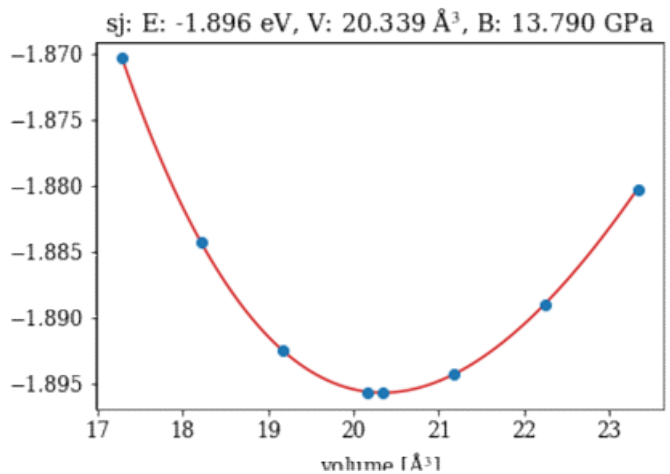
- 32 atoms => 8 cells [2*2*2]
- 108 atoms => 27 cells [3*3*3]

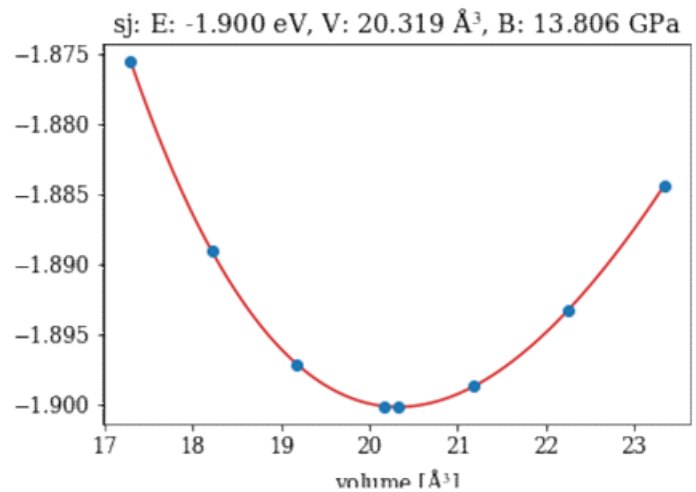
Structural data was taken from https://legacy.materialsproject.org/

Metals optimization

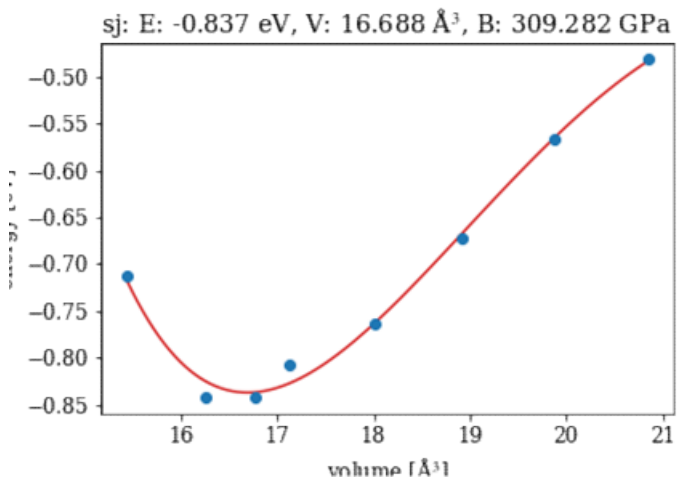
ENCUT 150 **ENCUT 300**

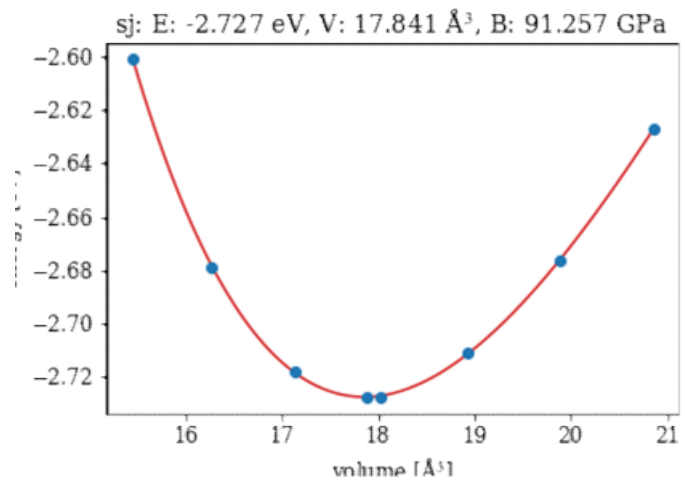
Li





Ag



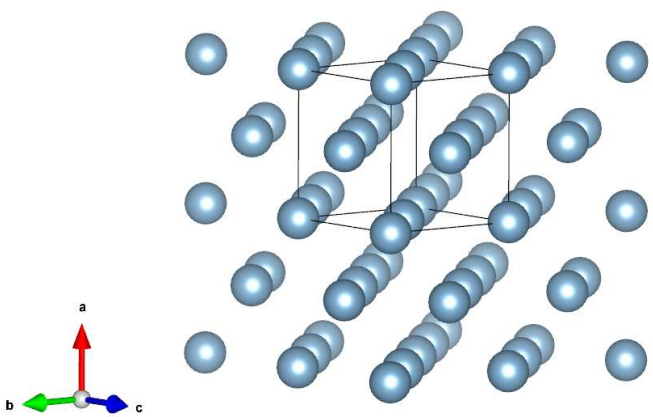


Vacancy

$E_{v(Experimental)}$ = 0.66 eV

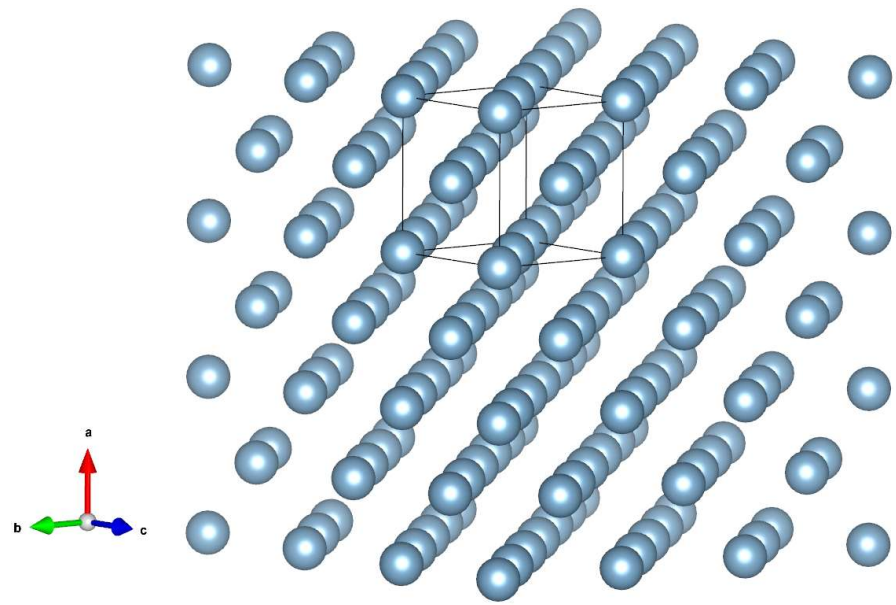
[2*2*2] – E_v = 0.69 eV

1/32 = 3.1%



[3*3*3] – E_v = 0.63 eV

1/108 = 0.9%



V_{vac} = 33 Å^3

$V_{sphere} \sim 4r_{met}^3$

r_{met} – 1.3 – 1.6 Å => V_{at} – 8.7 – 16.4 Å^3

M.J. Gillan // J. Phys.: Condens. Matter 1989

Vacancy

V_{vac} = 33 Å^3

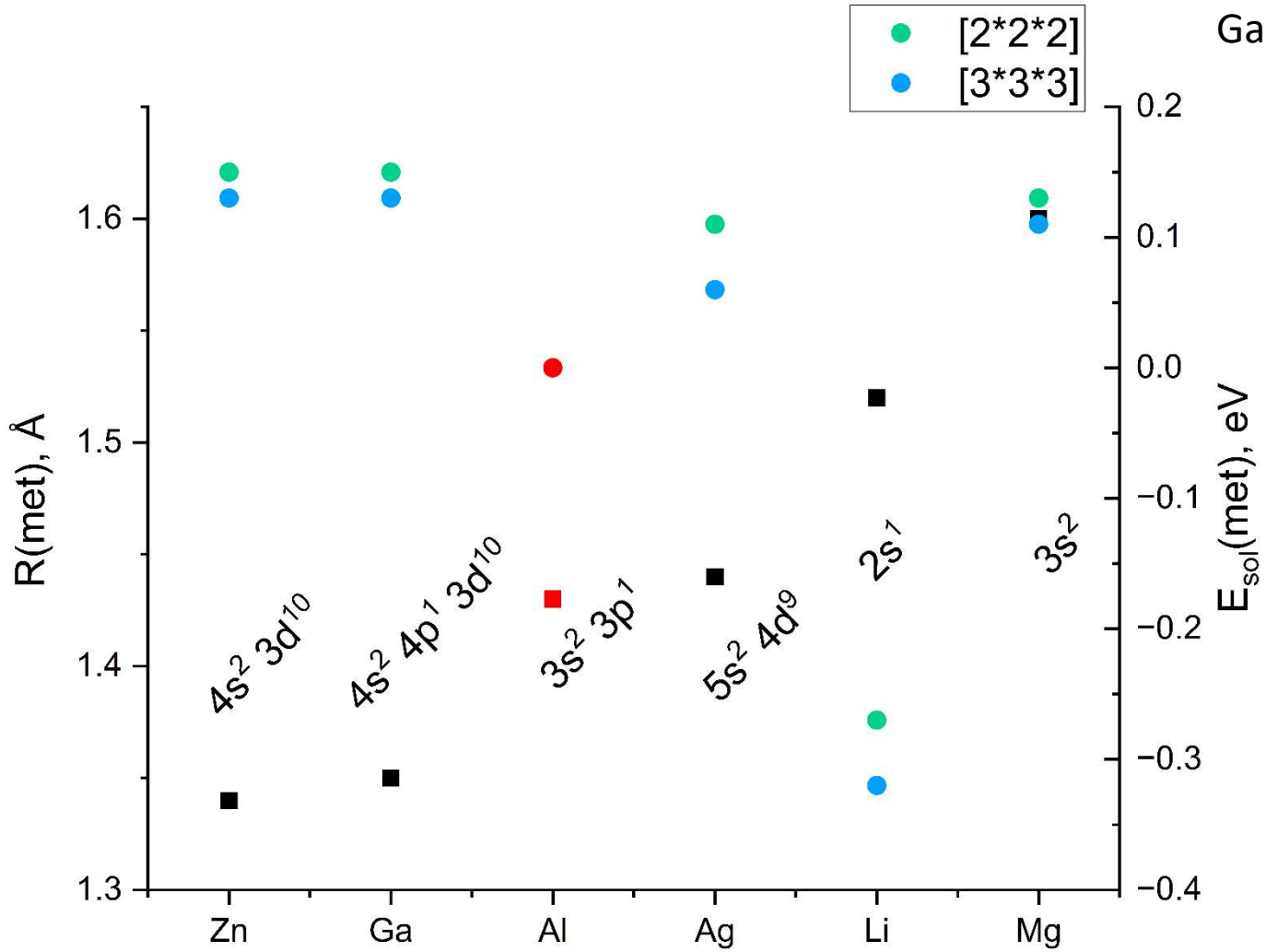
$V_{sphere} \sim 4r_{met}^3$ but T = 0 K

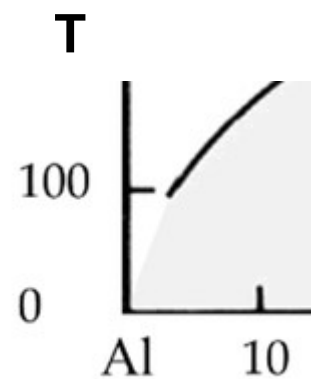
Mg, Zn – hcp

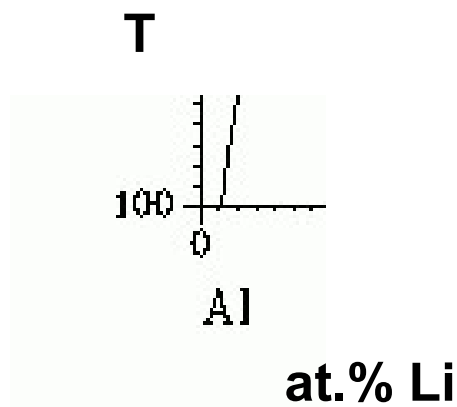
Al, Ag – ccp

Li – bcc

Ga – distorted hcp (Cmce)







https://www.researchgate.net

Binding energy

V_{vac} = 33 Å^3

$V_{sphere} \sim 4r_{met}^3$ but T = 0 K

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Al, Ag – ccp

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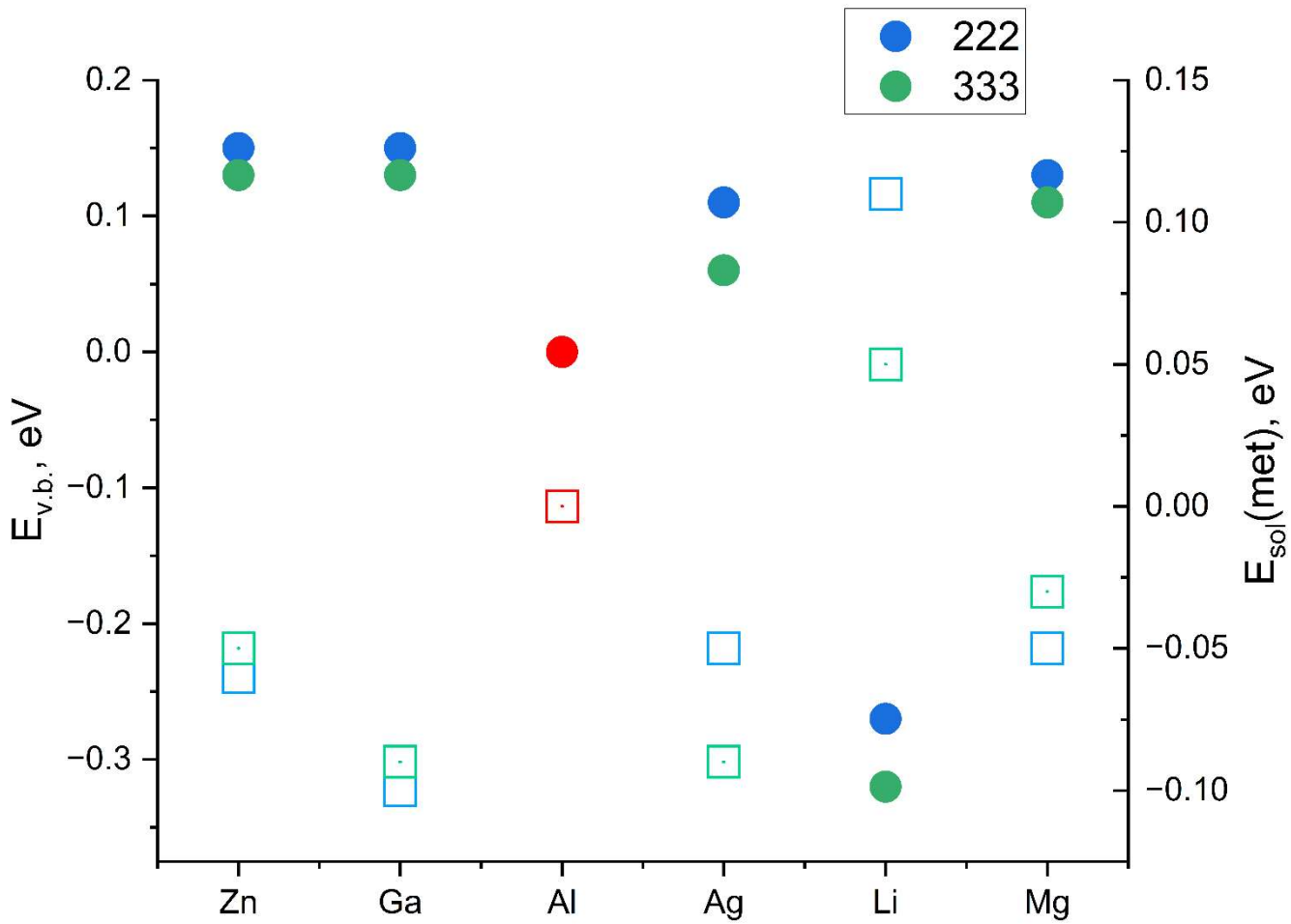

Migration barrier by NEB, eV

Zn	0.35
Ga	0.35
Al	0.60
Ag	0.41
Li	0.40
Mg	0.43