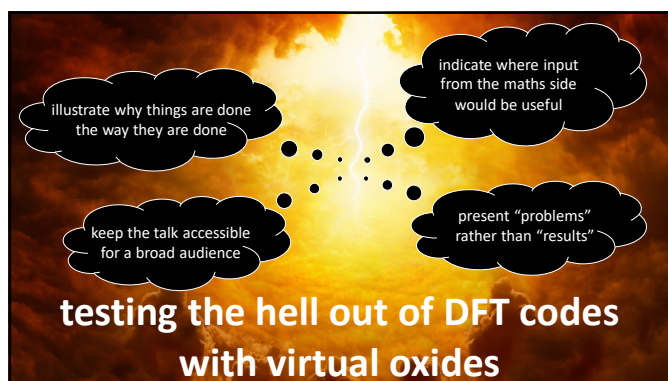




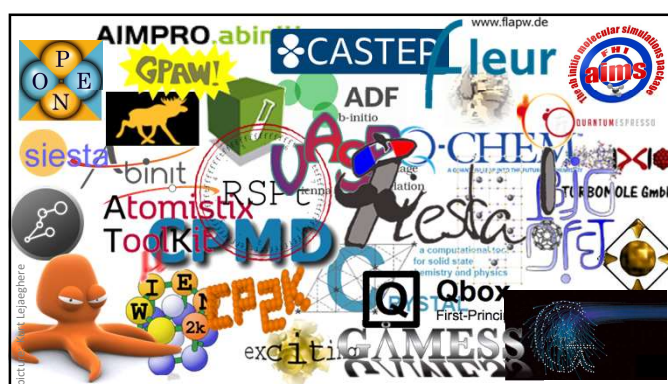
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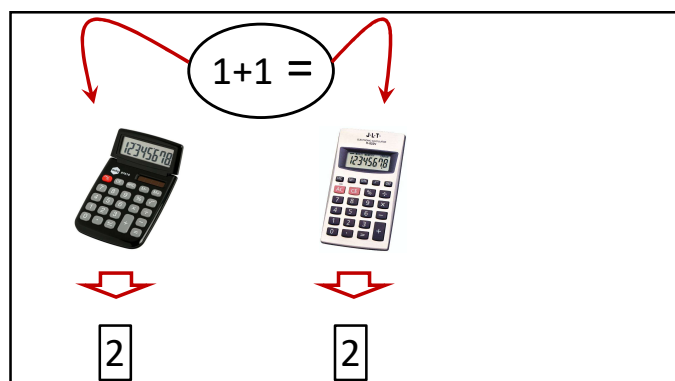
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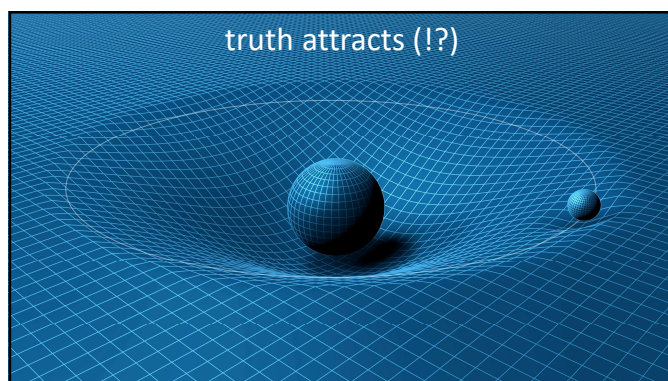
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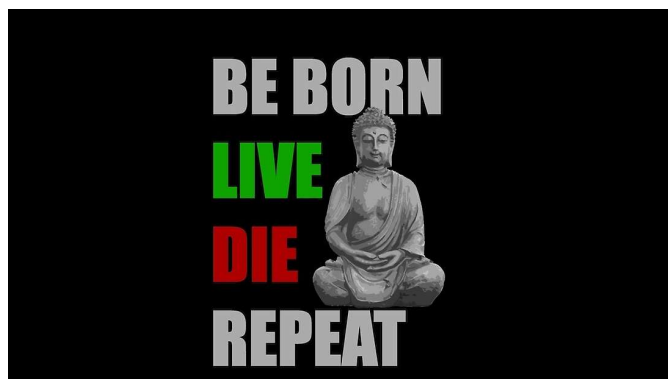
5



6



13



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Emanuele Bosoni,^{1,*} Louis Beal,² Marnik Berx,³ Peter Blaha,⁴ Stefan Blügel,⁵ Jens Brüder,^{5,6} Martin Callen,^{7,8,9} Stefan Cottenier,^{7,8} Augustin Degomme,² Vladimir Dikan,¹ Espen Flage-Larsen,^{10,11} Alberto Garcia,¹ Luigi Genovese,² Matteo Giantomassi,¹² Sebastiaan P. Huber,^{3,13} Henning Janssen,⁵ Georg Kaeuber,¹⁴ Matthias Krack,¹⁵ Thomas D. Kühne,¹⁶ Kurt Lejaeghere,^{5,17} Georg K. H. Madsen,⁴ Nicola Marzari,^{3,15} Gregor Michalek,⁵ Hossein Mirhosseini,¹⁶ Tiziano M. A. Müller,¹⁸ Guido Petretto,¹² Chris J. Pickard,¹⁹ Samuel Ponce,¹² Gian-Marco Rignanese,¹² Oleg Rubel,²⁰ Thomas Ruhl,^{4,8} Michael Sluydts,^{7,8,21} Danny E.P. Vanpoucke,^{7,22} Sudarshan Vijay,¹⁴ Michael Wlochow,^{23,24} Daniel Wortmann,⁵ Aliaksandr V. Yakutovich,²⁵ Austin Zadoks,³ Bonan Zhu,^{26,27} and Giovanni Pizzi¹

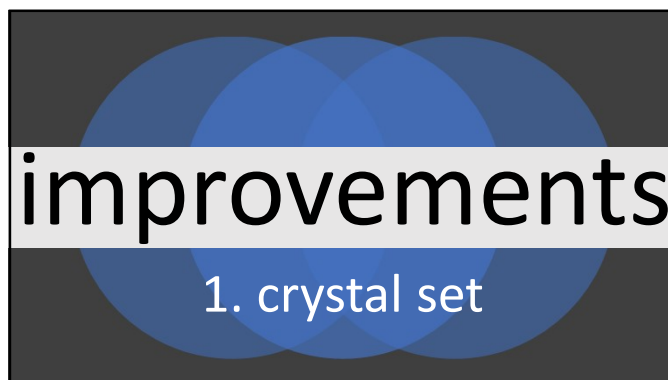


Emanuele Bosoni
ICMAB

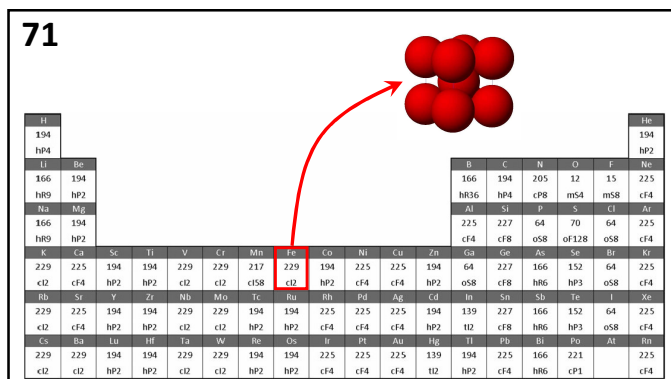


Giovanni Pizzi
EPFL

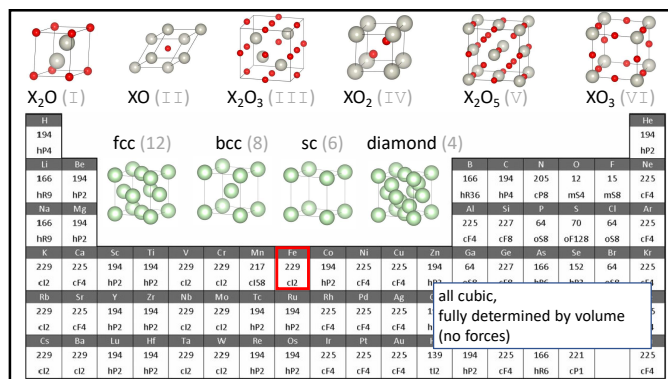
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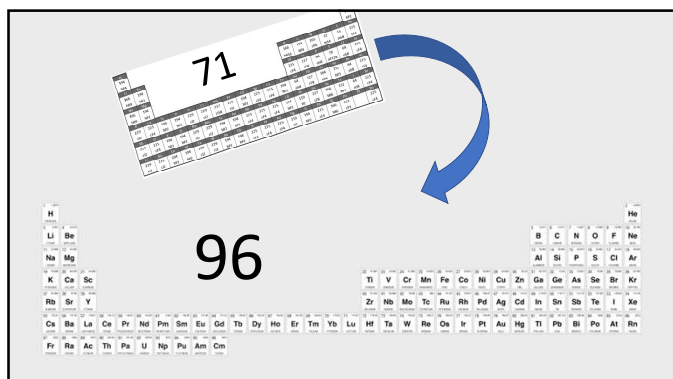
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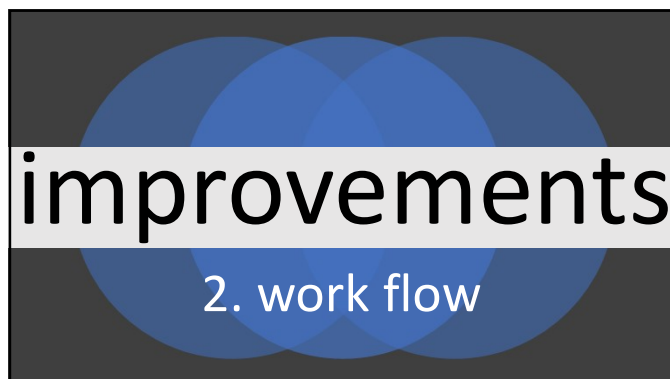
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18



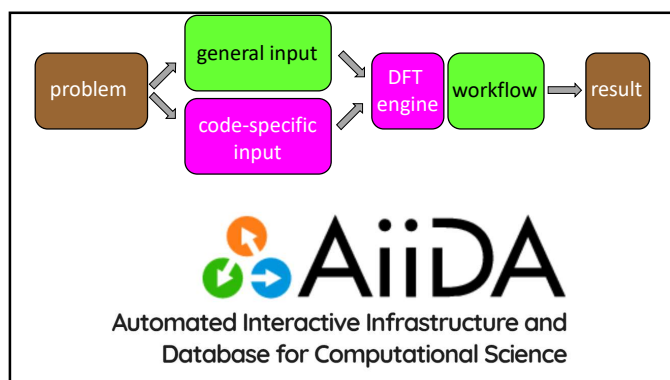
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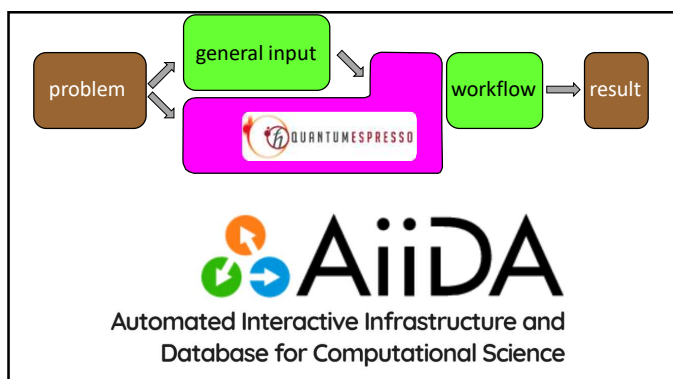
20

$96 \times 10 \times 7 = 6720$ static DFT calculations
with +10 codes

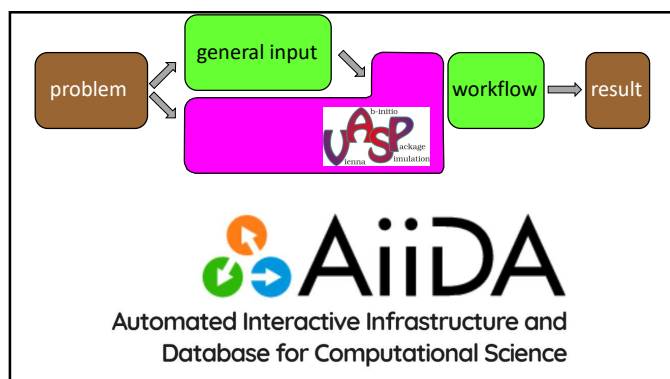
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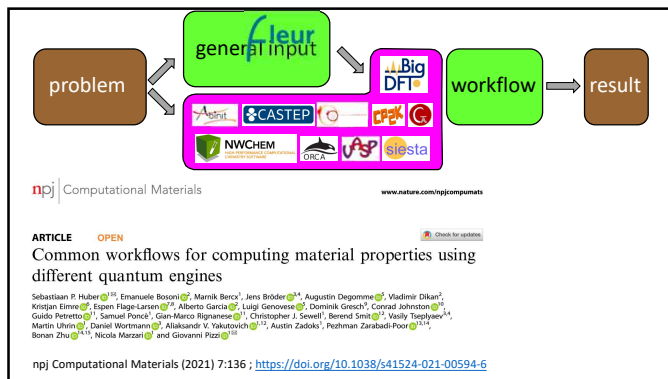
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23



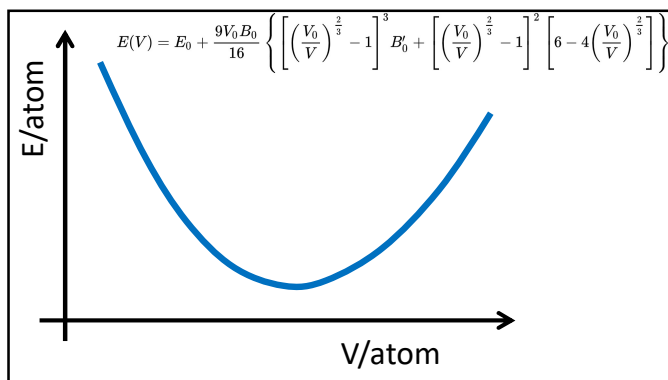
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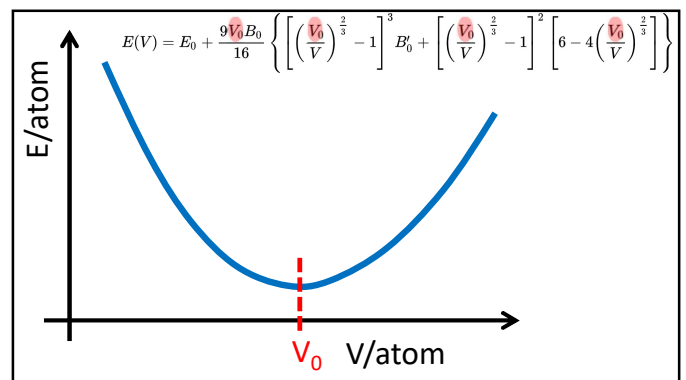
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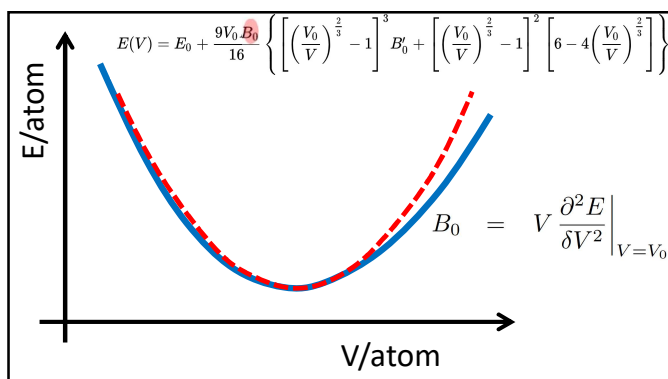
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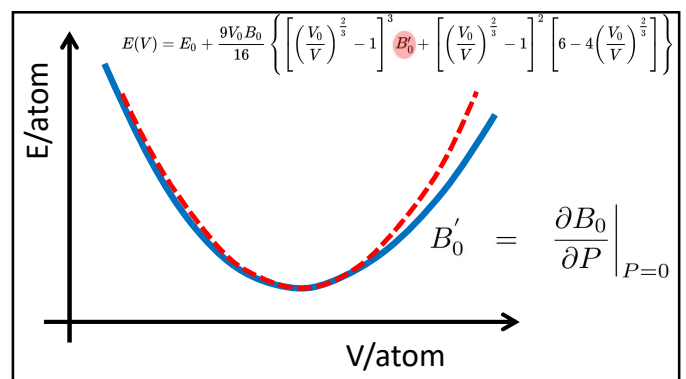
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28



29



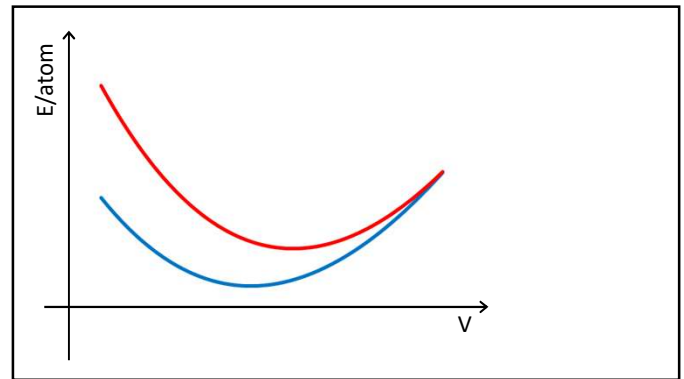
30

	E_0 (eV)	V_0 (Ång ³)	B_0 (GPa)	B_1
Al ₂ O	-658.8152	46.147	56.92	5.202
AlO	-550.6173	22.421	133.41	3.991
Al ₂ O ₃	-3088.9433	98.326	186.79	4.091
AlO ₂	-991.0037	26.254	208.27	4.061
Al ₂ O ₅	-4820.2194	125.859	172.18	4.231
AlO ₃	-1426.5734	49.675	121.99	4.102

Al ₂ O	-573.6487	46.021	57.26	5.237
AlO	-513.2723	22.366	133.90	4.028
Al ₂ O ₃	-2960.5872	98.024	186.71	4.078
AlO ₂	-964.1461	26.187	208.25	4.093
Al ₂ O ₅	-4733.6112	125.679	172.51	4.200
AlO ₃	-1410.1697	49.571	121.77	4.180

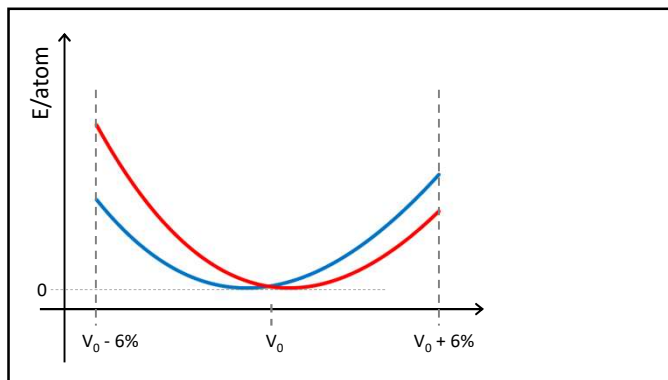
CASTEP

Abinit

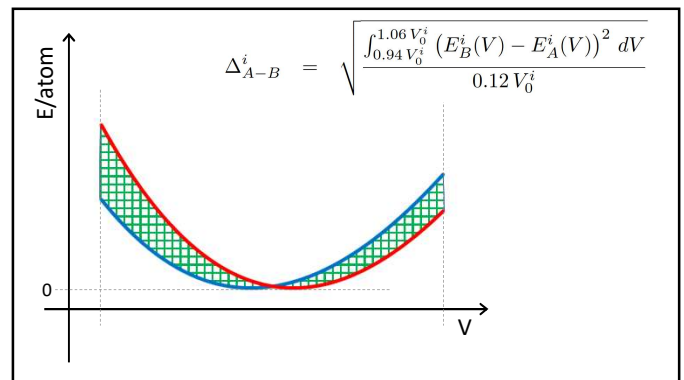


31

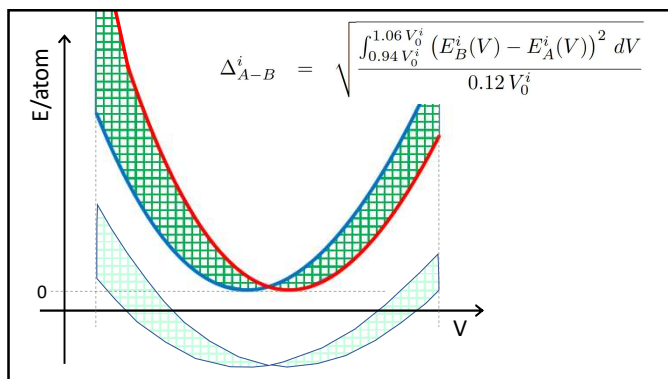
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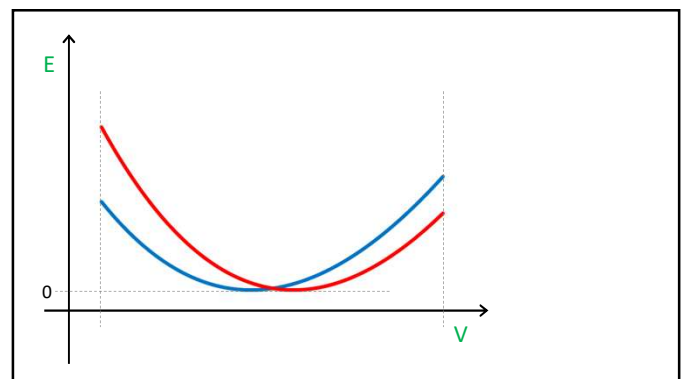
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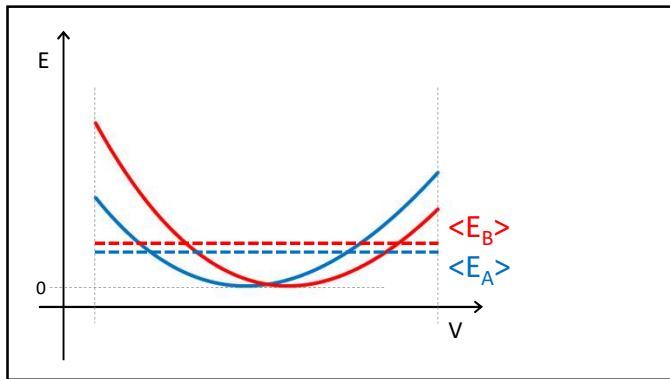
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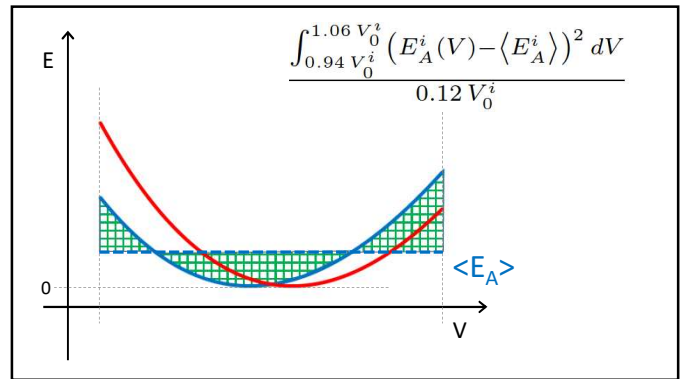
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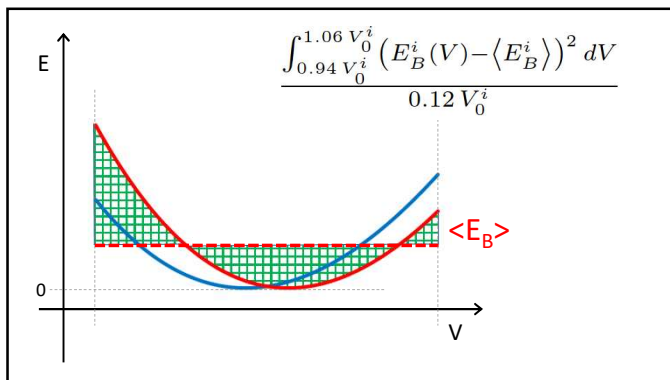
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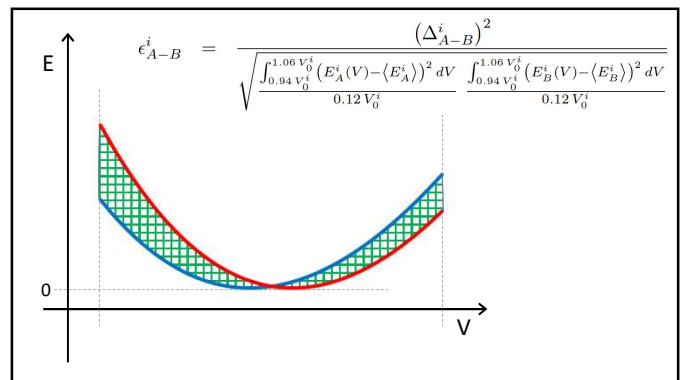
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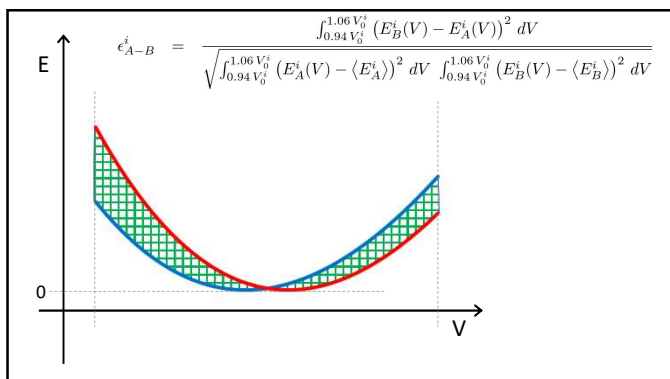
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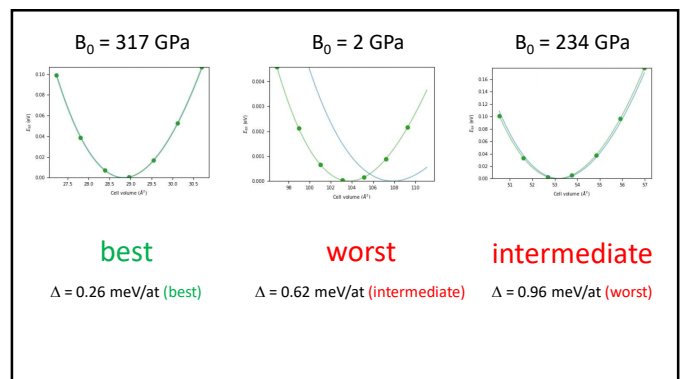
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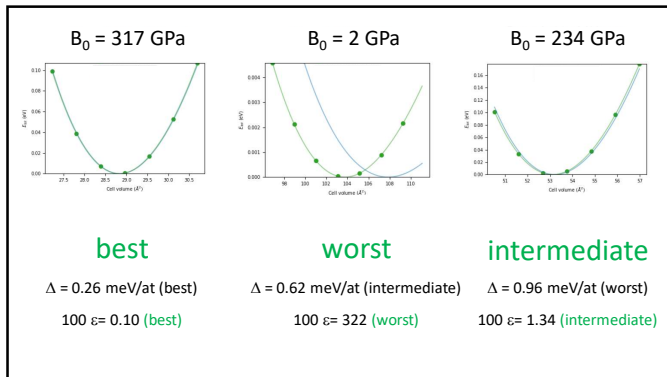
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41



42

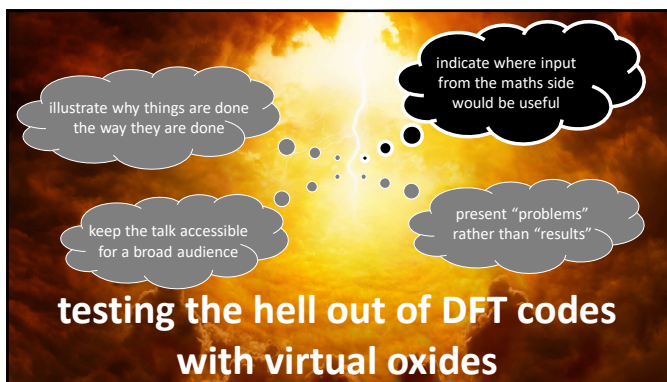


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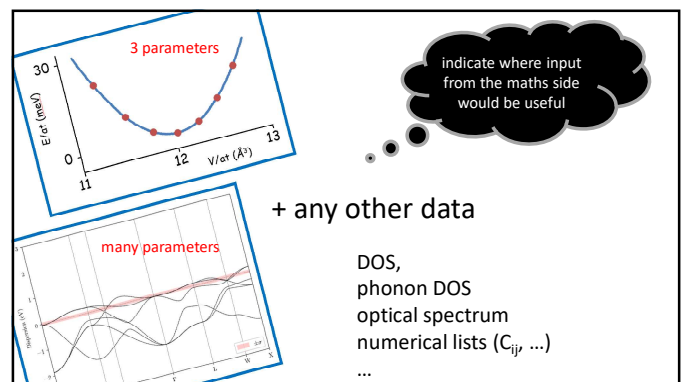
$$\nu_{A-B}^i = \sqrt{\sum_P \left(w_P \frac{P_A - P_B}{\frac{P_A + P_B}{2}} \right)^2}$$

$$\frac{V_0(A) - V_0(B)}{V_0(A) + V_0(B)}$$

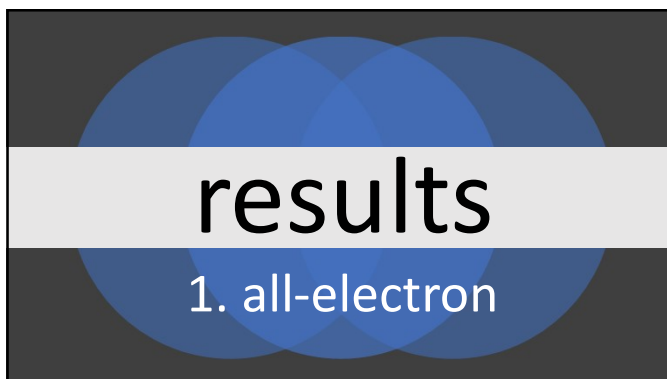
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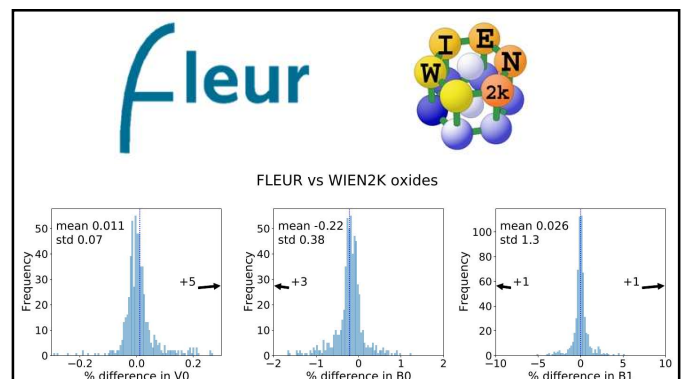
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46



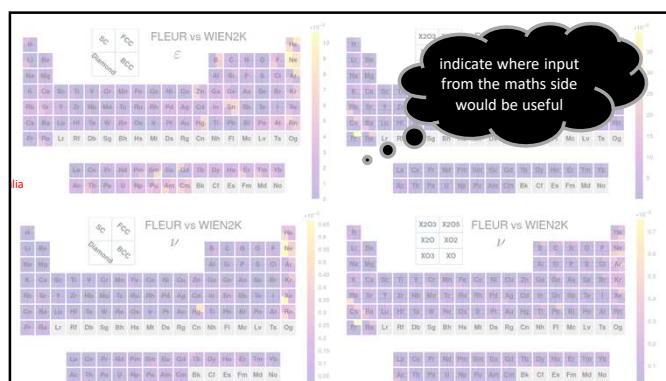
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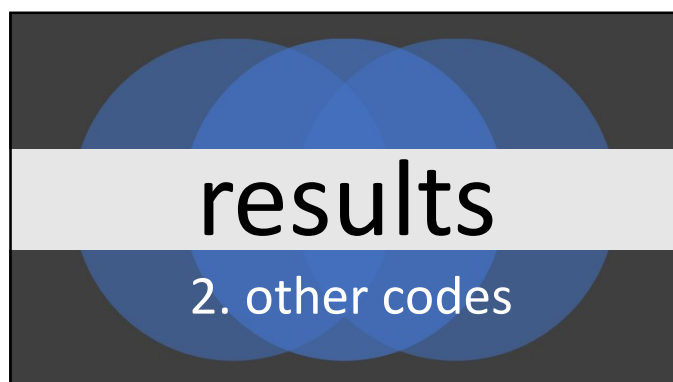
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49



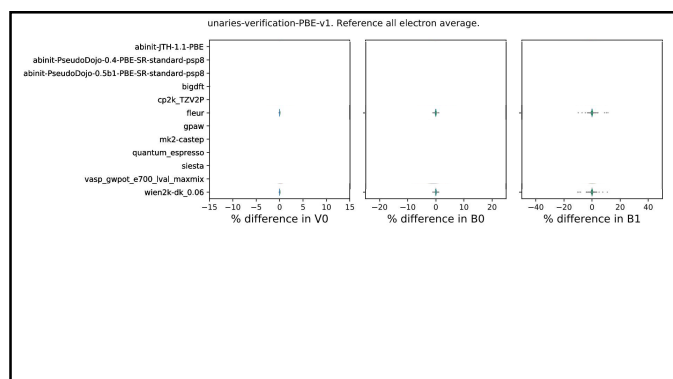
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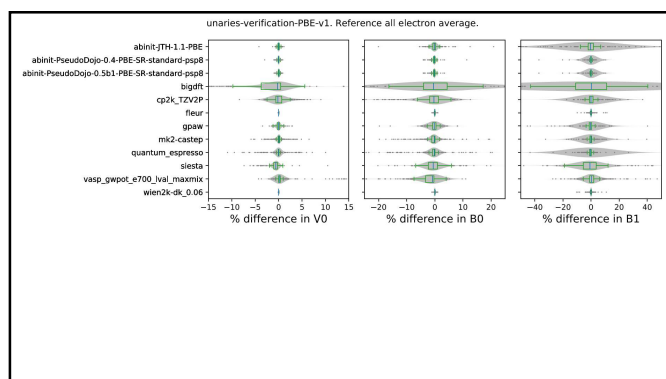
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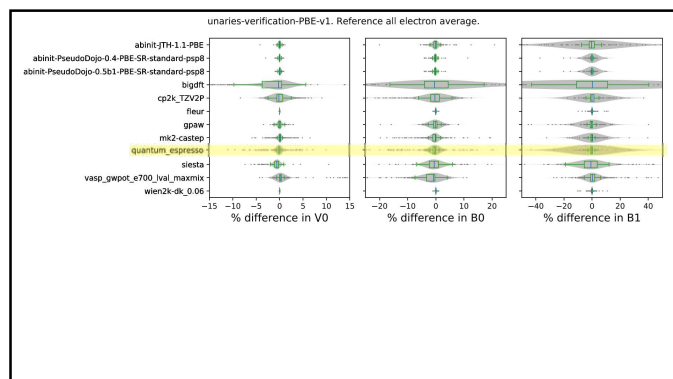
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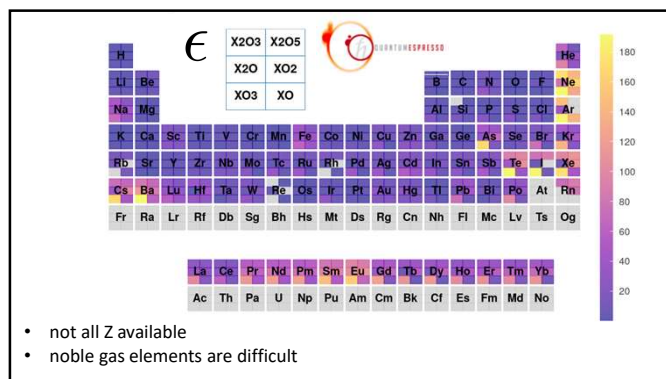
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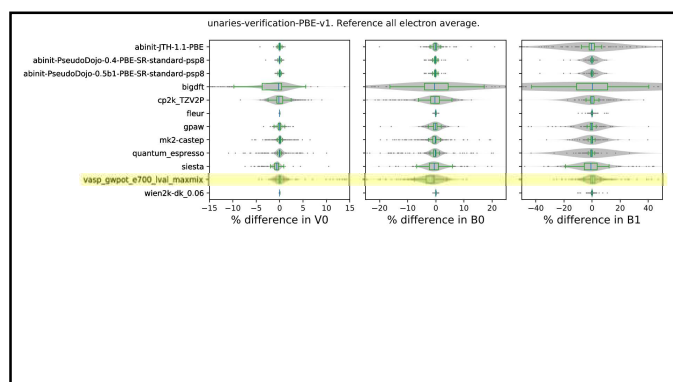
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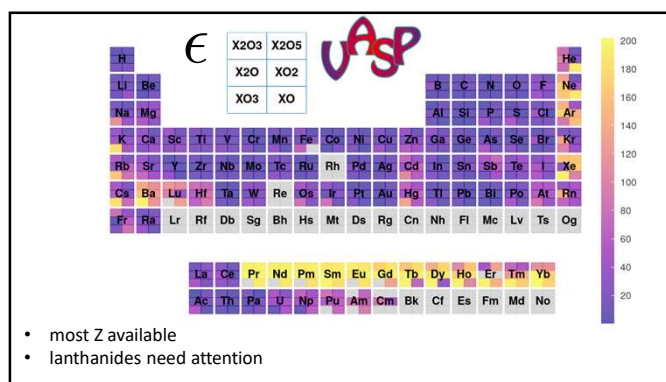
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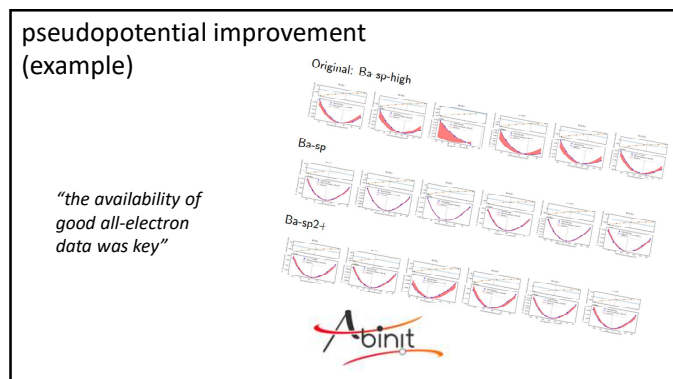
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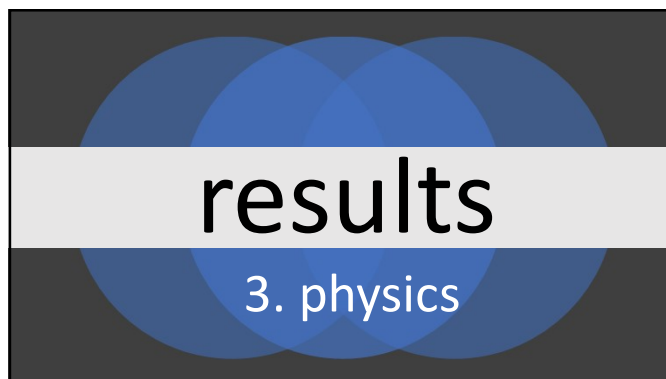
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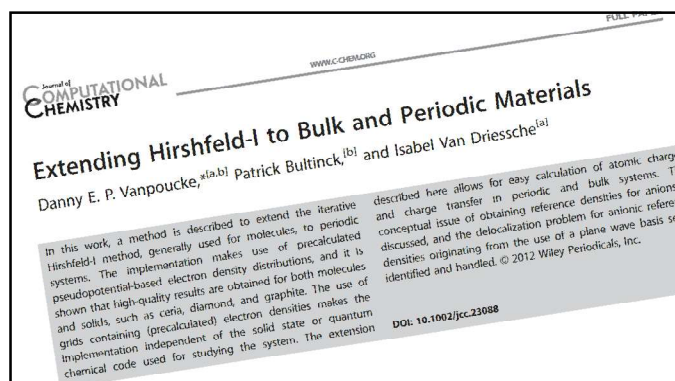
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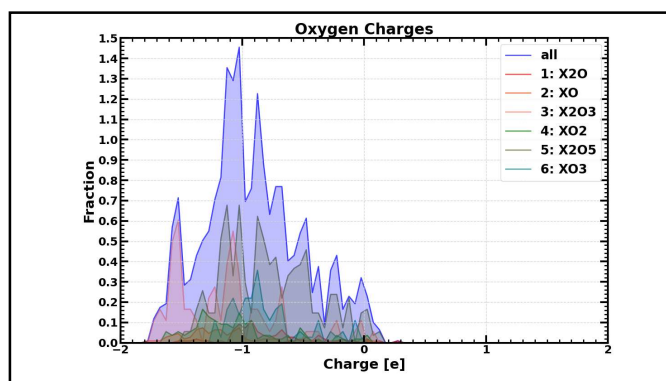
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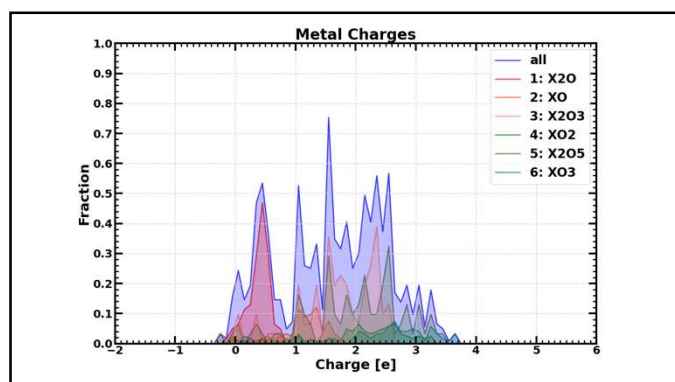
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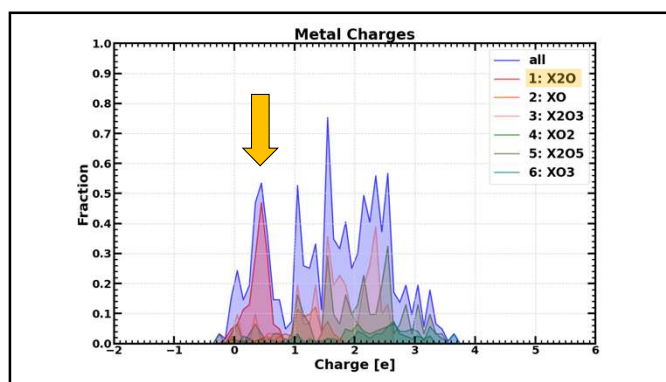
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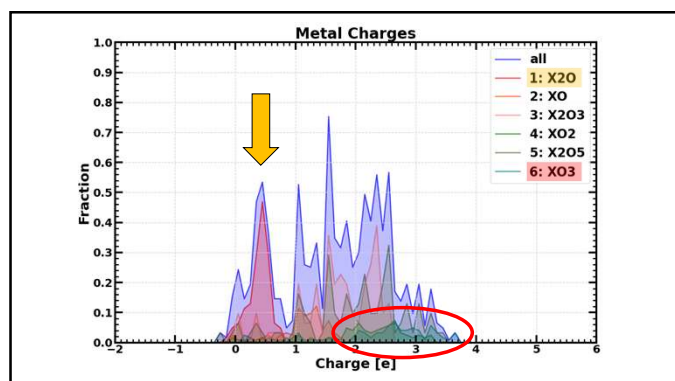
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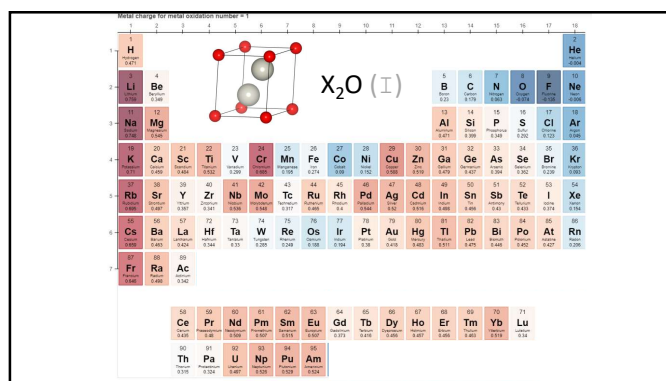
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64



65

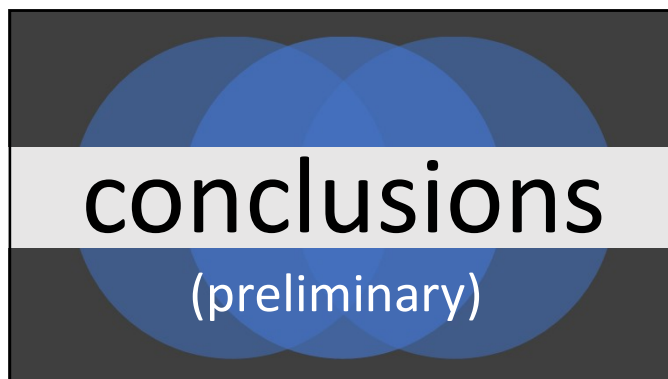


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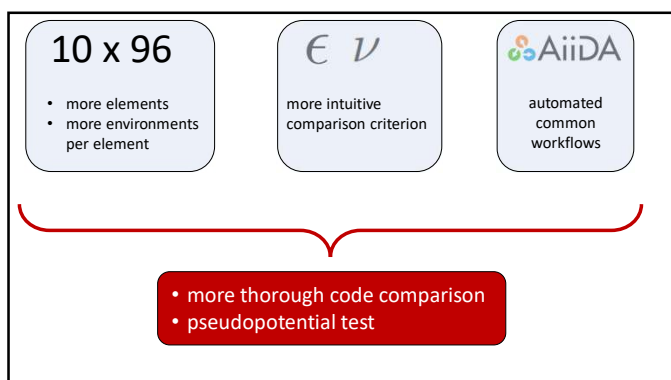
Metals change for metal oxidation number = 0

The image shows a periodic table with a diagram of a crystal lattice structure. The chemical formula $XO(II)$ is highlighted in the center. The periodic table includes elements from Hydrogen (H) to Oganesson (Og), with various element symbols and atomic numbers.

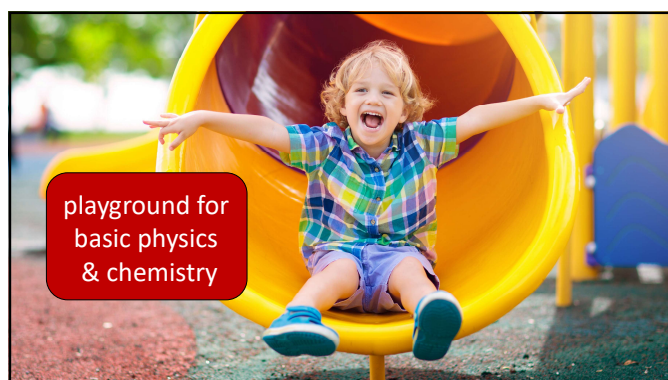
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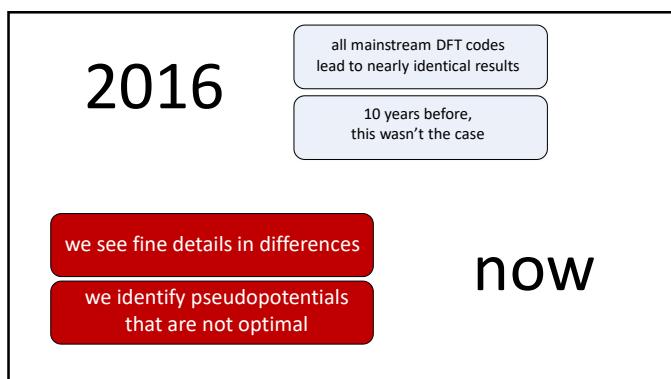
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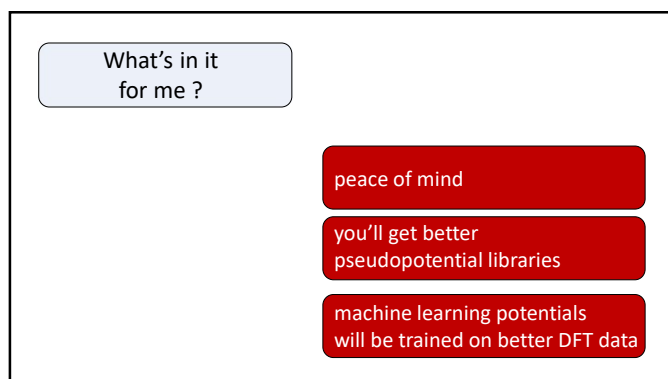
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What's in it for me ?

indicate where input from the maths side would be useful

- comparison tools ?
- DFTK ? 
- ...

peace of mind

you'll get better pseudopotential libraries

machine learning potentials will be trained on better DFT data

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Emanuele Bosoni,^{1,*} Louis Beal,² Marnik Berx,³ Peter Blaha,⁴ Stefan Blügel,⁵ Jens Brüder,^{5,6} Martin Calsen,^{7,8,9} Stefaan Cottenier,^{7,8} Augustin Degomme,² Vladimir Dikan,¹ Espen Flage-Larsen,^{10,11} Alberto Garcia,¹ Luigi Genovese,² Matteo Giantomassi,¹² Sebastiaan P. Huber,^{3,13} Henning Janssen,⁵ Georg Kastlunger,¹⁴ Matthias Krack,¹⁵ Thomas D. Kühne,¹⁶ Kurt Lejaeghere,^{8,17} Georg K. H. Madsen,⁴ Nicola Marzari,^{3,15} Gregor Michalíček,⁵ Hossein Mirhosseini,¹⁶ Tiziano M. A. Müller,¹⁸ Guido Petretto,¹² Chris J. Pickard,¹⁹ Samuel Poncé,¹² Gian-Marco Rignanese,¹² Oleg Rubel,²⁰ Thomas Rühl,^{4,8} Michael Shuydts,^{7,8,21} Danny E.P. Vanpoucke,^{7,22} Sudarshan Vijay,¹⁴ Michael Wlochow,^{23,24} Daniel Wortmann,⁵ Aliaksandr V. Yakutovich,²⁵ Austin Zadoks,³ Bonan Zhu,^{26,27} and Giovanni Pizzi^{3,†}

with collaboration, you do MORE !




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