Fine-tuning Stability of La-Ni-Sn-H Materials for Hydrogen Storage

Martin Friák[1], Sabina Kovaříková Oweis[1,2], Kateřina Dočkalová[1,2], Anna Huňařová[1,2], Jana Pavlů[2,1], Ondřej Zobač[1], David Holec[3], Monika Kawuloková[4], Simona Zlá[4], Bedřich Smetana[4]

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[4] Department of Chemistry and Physico-Chemical Processes, Faculty of Materials Science and Technology, VSB Technical University of Ostrava, Ostrava, Czech Republic;

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Czech Academy of Sciences, Žižkova 22, Brno 61600, Czech Republic

- IT4I Project(s) (5 minutes): Dedicate approximately 5 minutes to provide insights into your computational approach and methods. Discuss software utilisation, job sizes, parallelisation techniques, and the extent of computational resources employed. Sharing your computational experience will provide valuable context for the audience.
- Research (10 minutes): Allocate around 10 minutes to delve into your research endeavours. Highlight key findings, address challenges encountered, and emphasise the significance of your work. This segment should offer a concise yet comprehensive overview of your research area.
- Discussion (5 minutes): Please reserve 5 minutes to engage with questions and discussions from the audience.

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Our current project

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Materials and technologies for sustainable development

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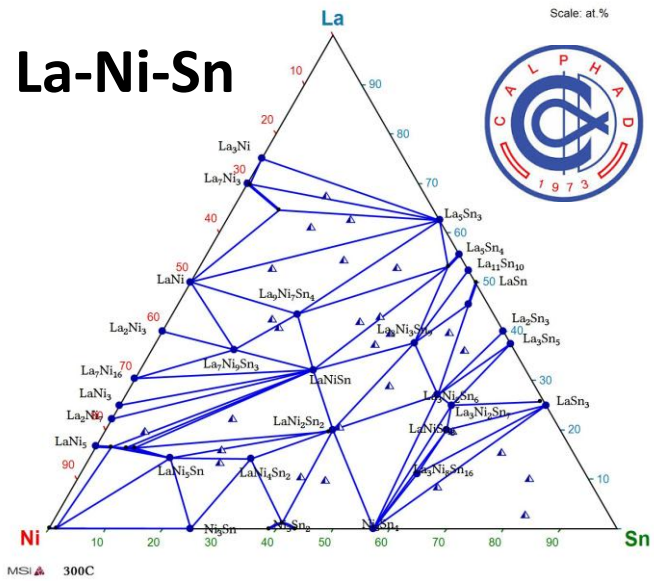
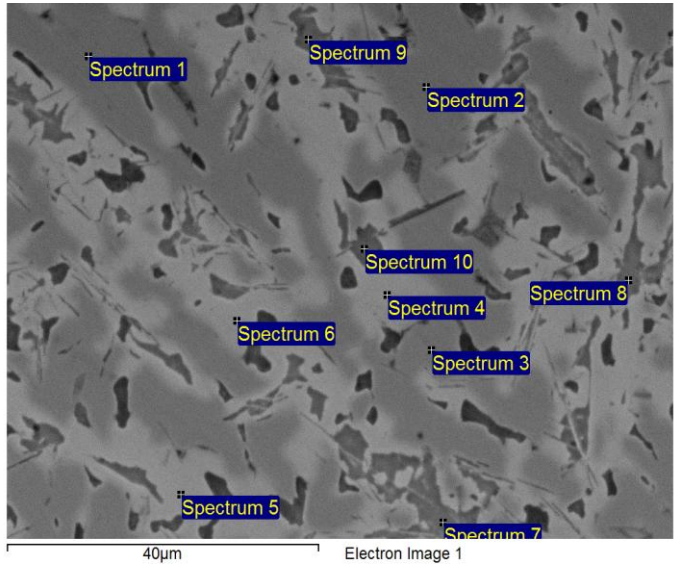
La-Ni-Sn





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Complexity of La-Ni-Sn (+H) phase diagram

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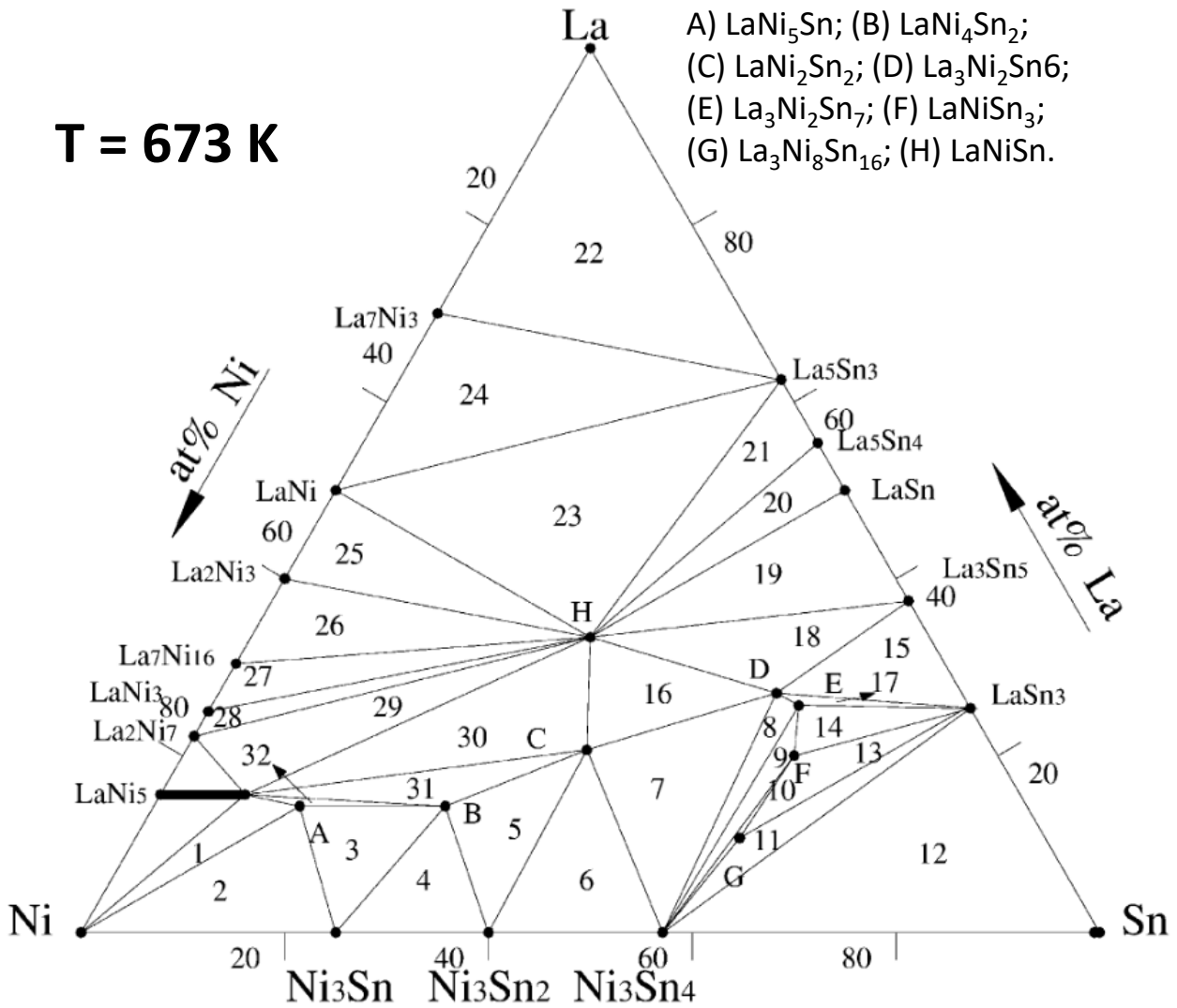
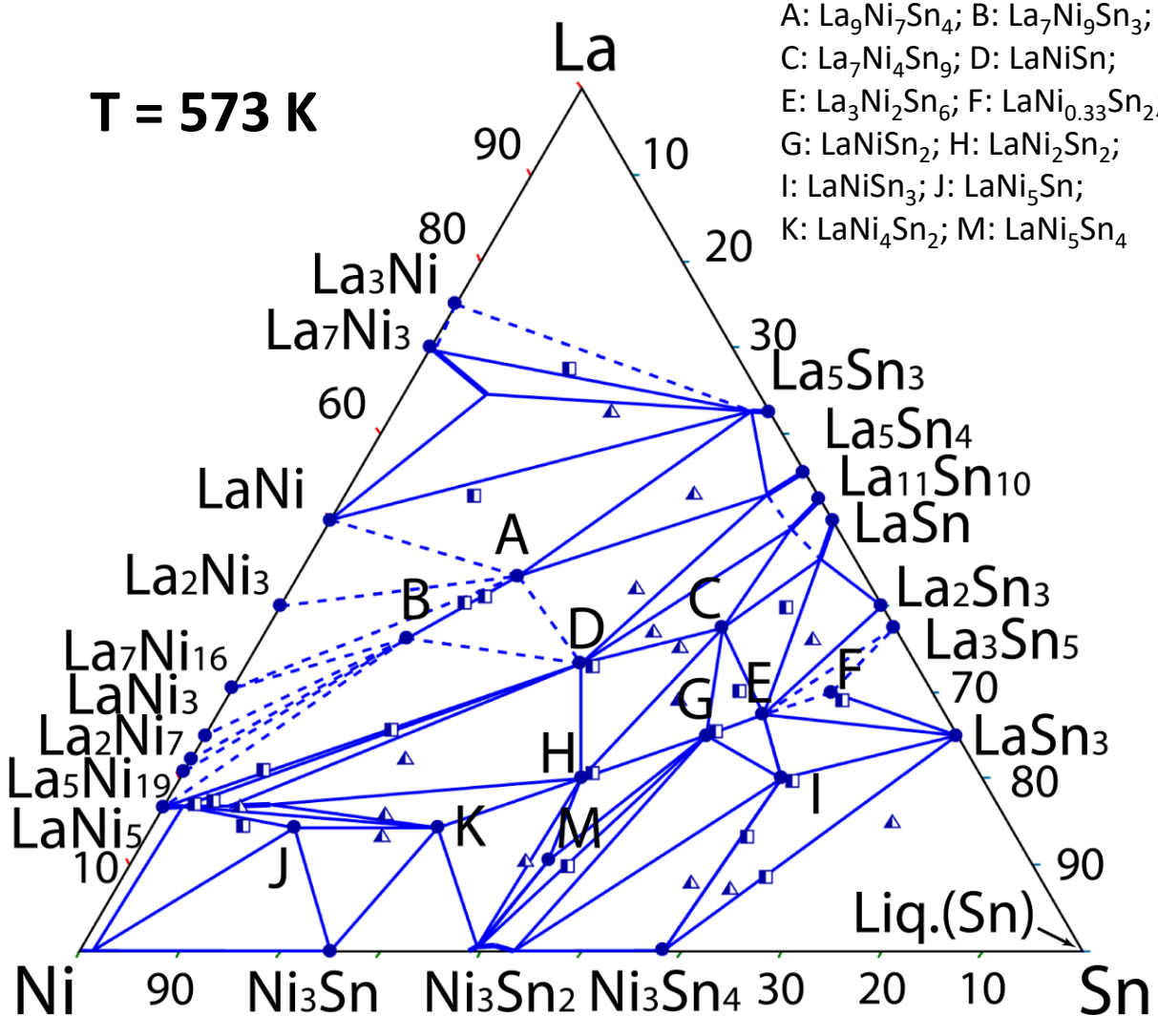


Y. Zhuang *et al.*, J. of Alloys and Comps. 363 (2004) 228.



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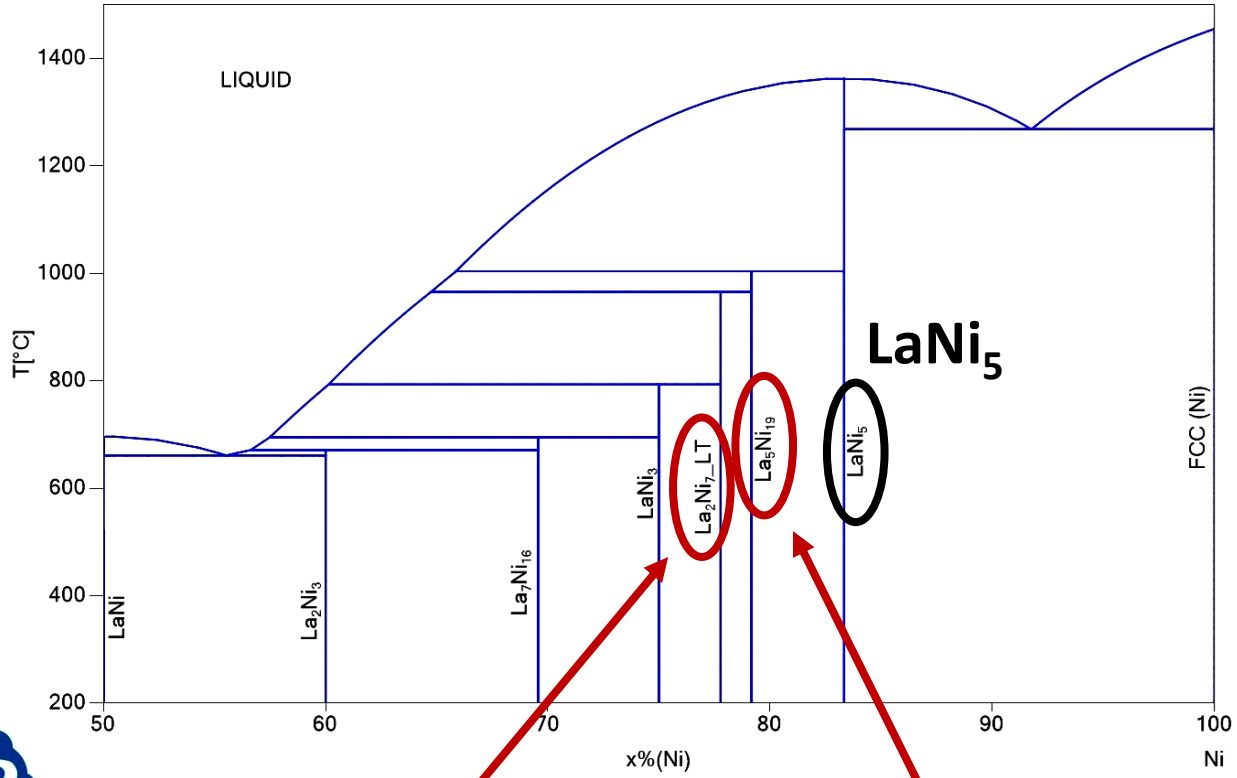
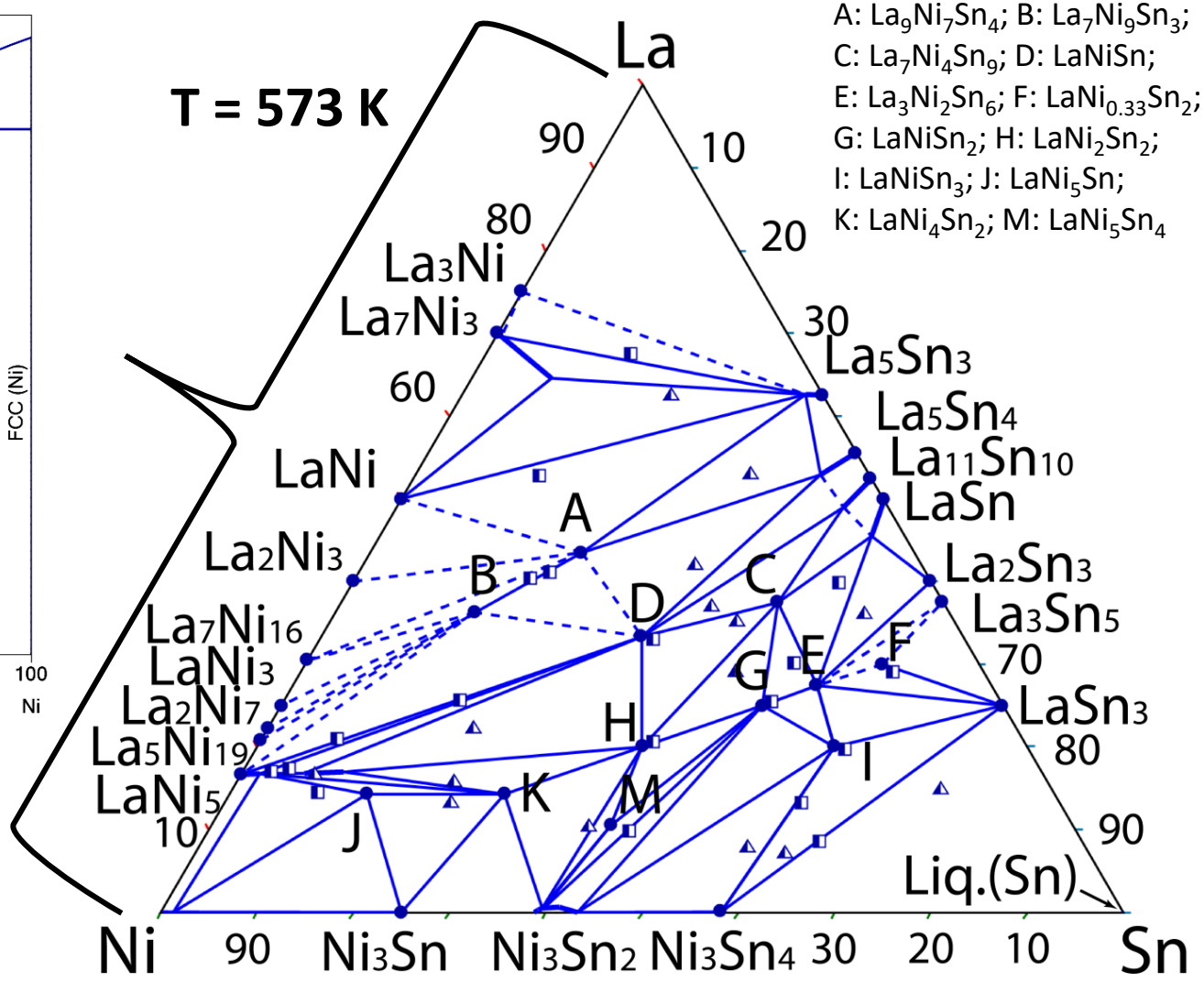


$LaNi_5$

La_2Ni_7 unknown stability

La_5Ni_{19} unclear structure



A: $La_9Ni_7Sn_4$; B: $La_7Ni_9Sn_3$;
C: $La_7Ni_4Sn_9$; D: LaNiSn;
E: $La_3Ni_2Sn_6$; F: $LaNi_{0.33}Sn_2$;
G: $LaNiSn_2$; H: $LaNi_2Sn_2$;
I: $LaNiSn_3$; J: $LaNi_5Sn$;
K: $LaNi_4Sn_2$; M: $LaNi_5Sn_4$

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Solubility of Sn in $LaNi_5$

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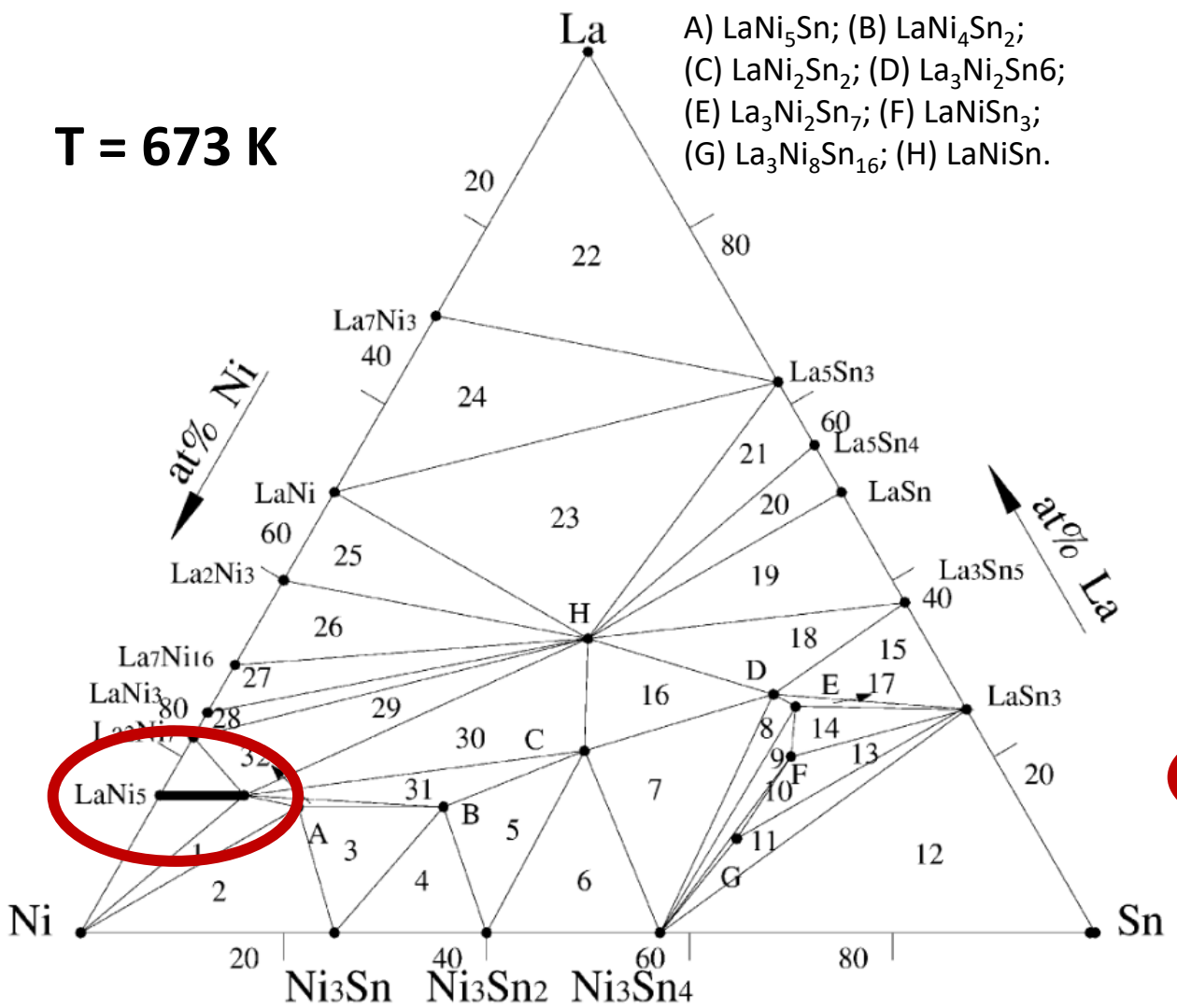

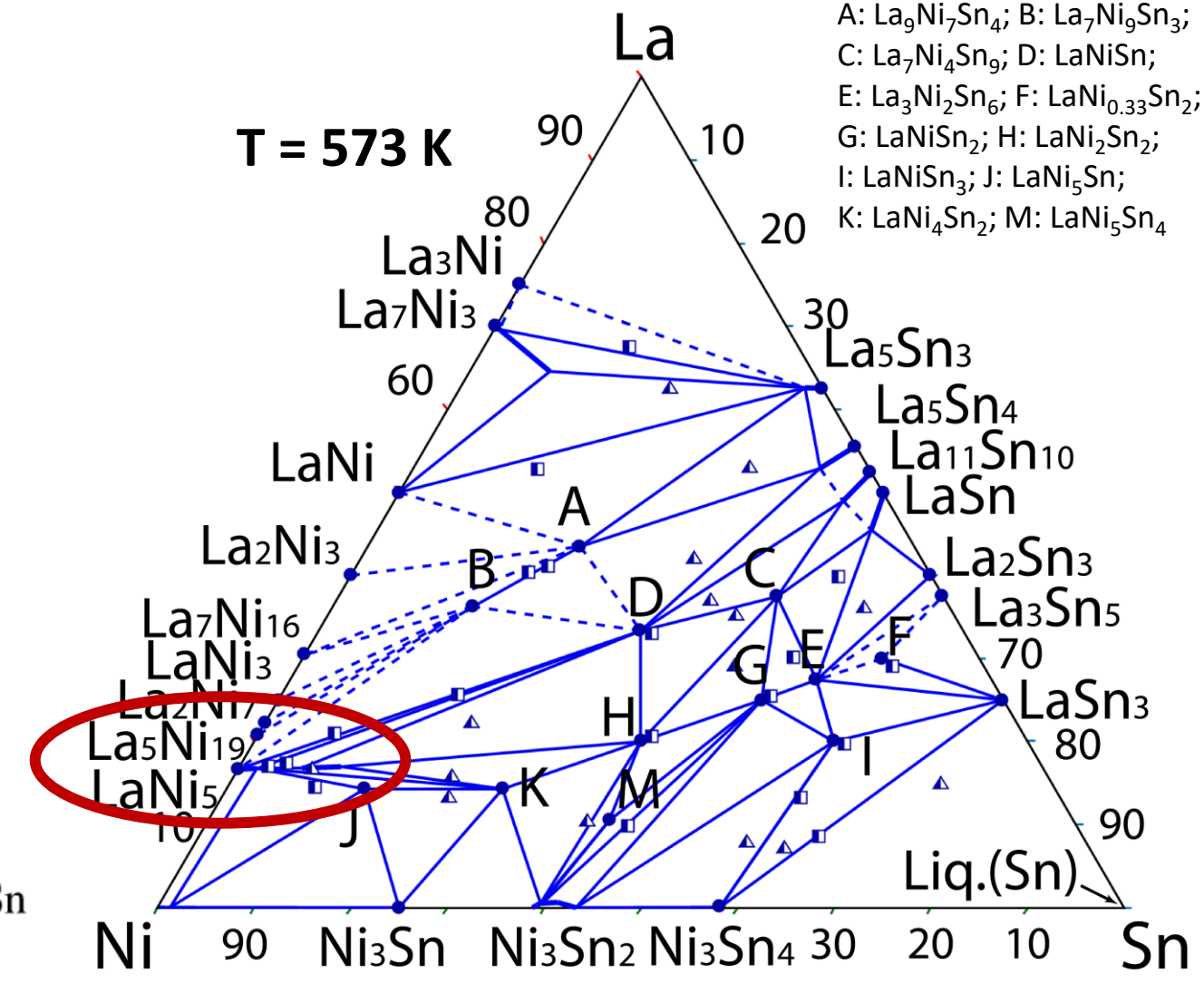

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Stability of $La(Ni,Sn)_5$: *ab initio* study

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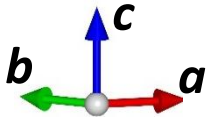
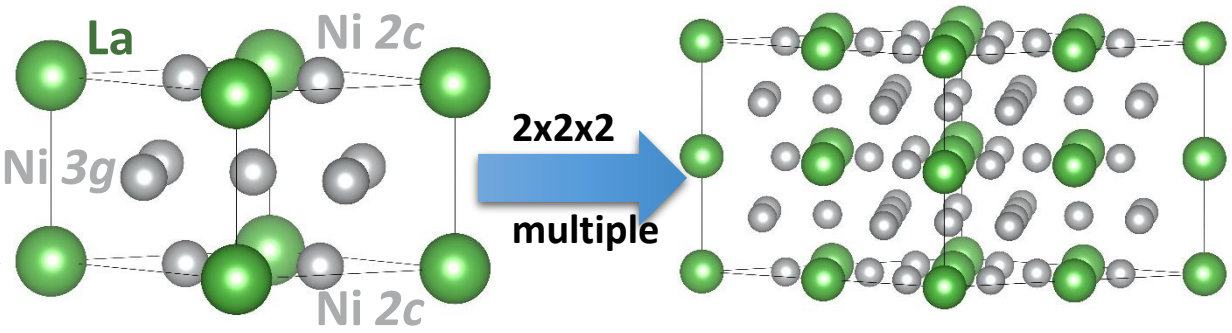
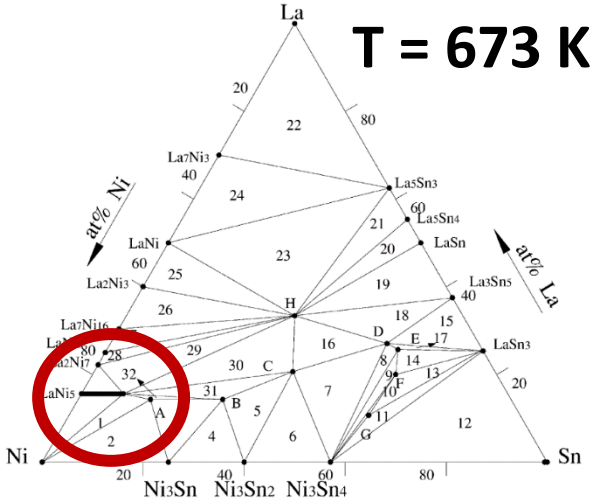
$LaNi_5$: hexagonal *P6/mmm* cell with *3g* and *2c* Ni sites





Sn atoms substituting Ni atoms are computed in 48-atom cell



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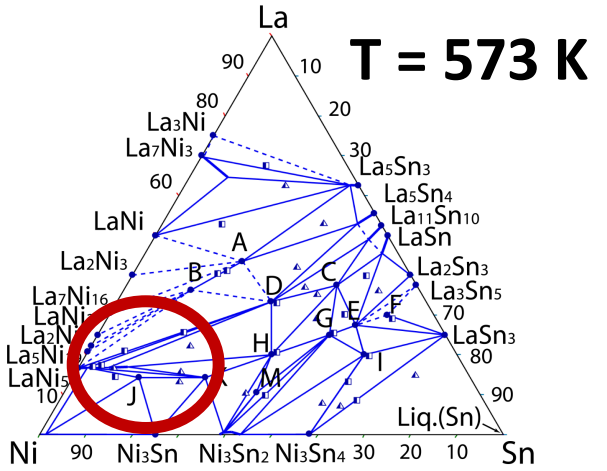

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Parameters of our quantum-mechanical calculations: the VASP code, Density Functional Theory (DFT), k-points: 12x12x16 and 6x6x8, the Generalized Gradient Approximation (GGA), 520 eV cut-off energy, the Projector Augmented Waves (PAW) potentials.

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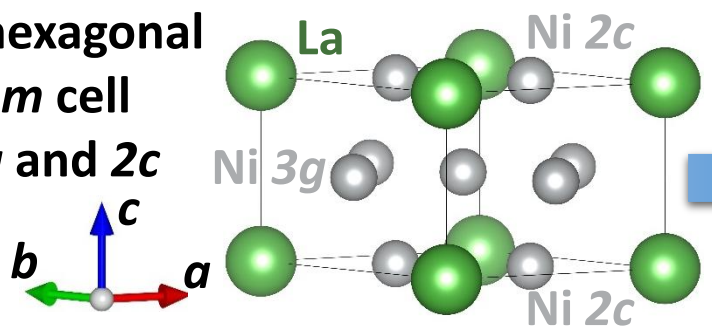

2x2x2 multiple

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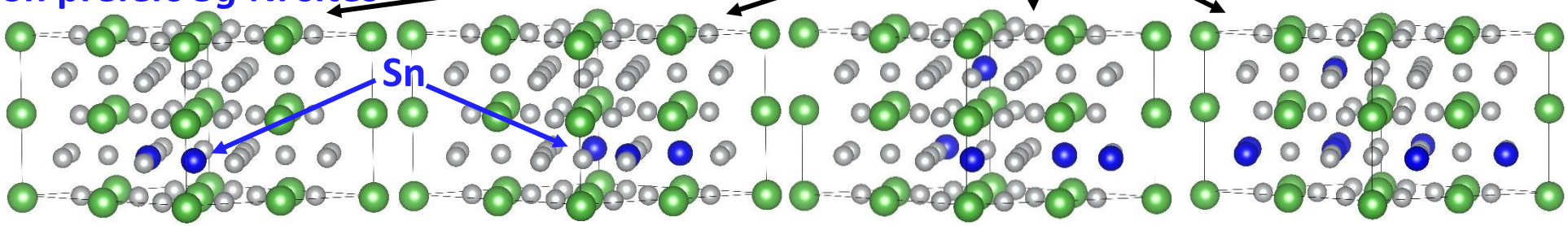
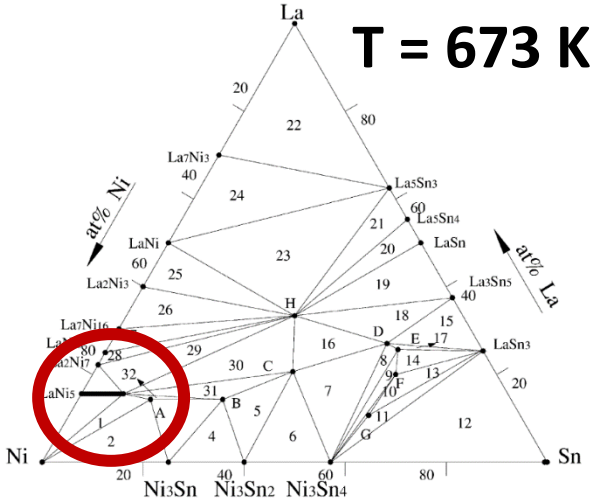


T = 673 K



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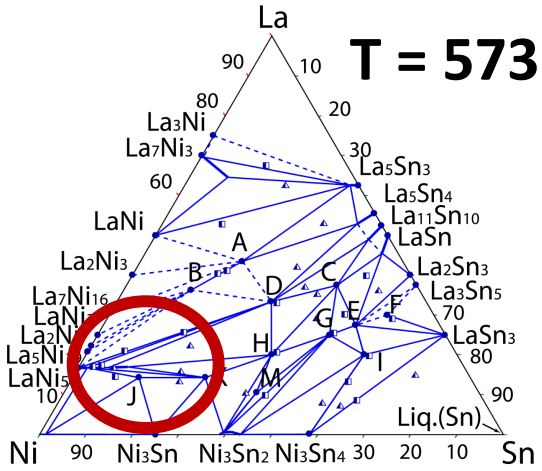
T = 573 K



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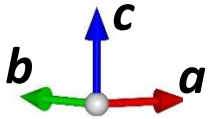
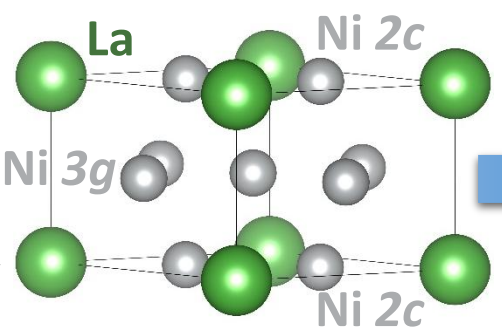
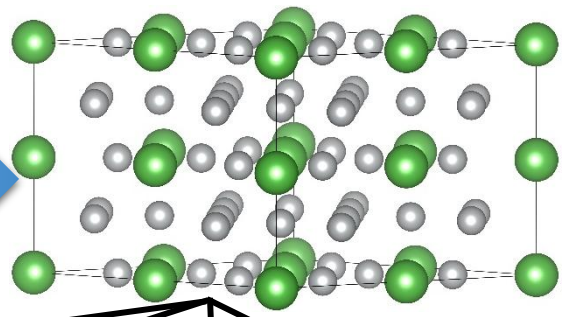




2x2x2 multiple



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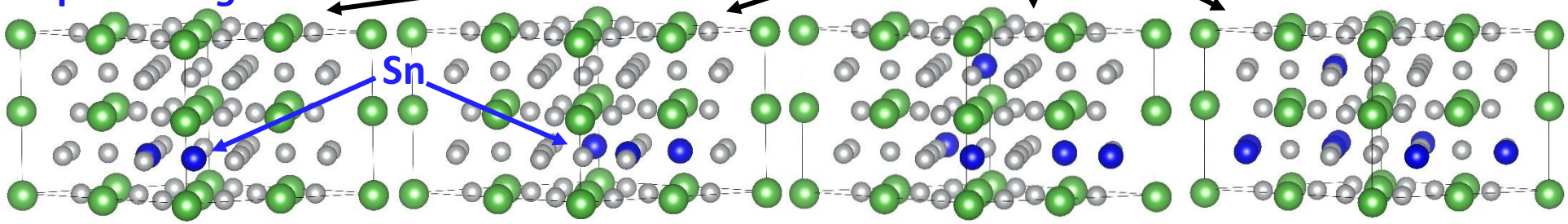

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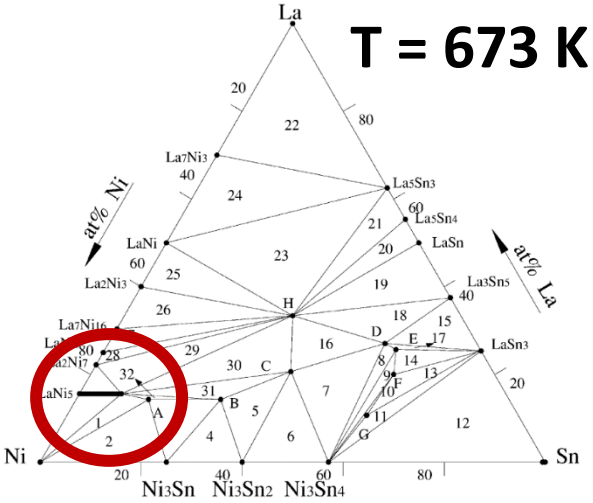

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$$E_{\text{formation}} = \frac{E(La(Ni_{1-x},Sn_x)_5) - x \cdot E(LaNi_5) - (1-x) \cdot E(LaSn_5)}{\text{number of atoms}}$$

Parameters of our quantum-mechanical calculations: the VASP code, Density Functional Theory (DFT), k-points: 12x12x16 and 6x6x8, the Generalized Gradient Approximation (GGA), 520 eV cut-off energy, the Projector Augmented Waves (PAW) potentials.

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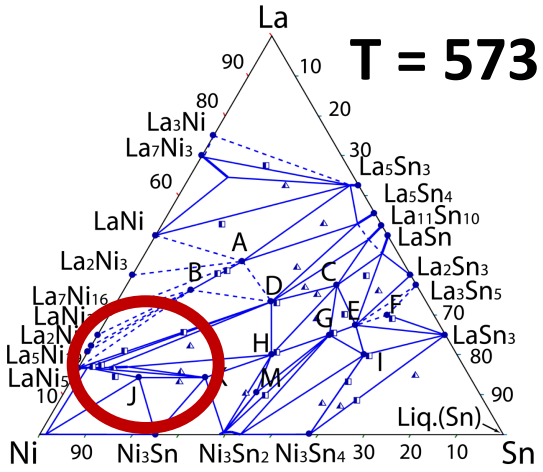

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From $LaNi_5$ to $LaSn_5$

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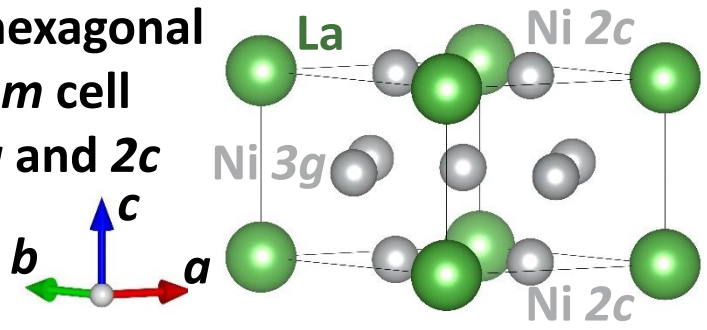
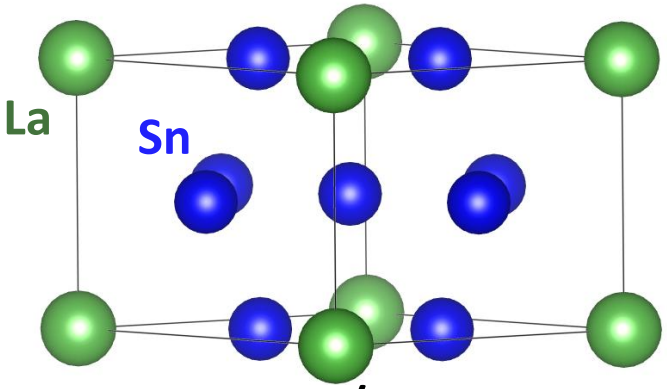
CALPHAD motivation: From $LaNi_5$ to $LaSn_5$

MATUR

$LaNi_5$: hexagonal *P6/mmm* cell with *3g* and *2c* Ni sites



Full Sn substitution



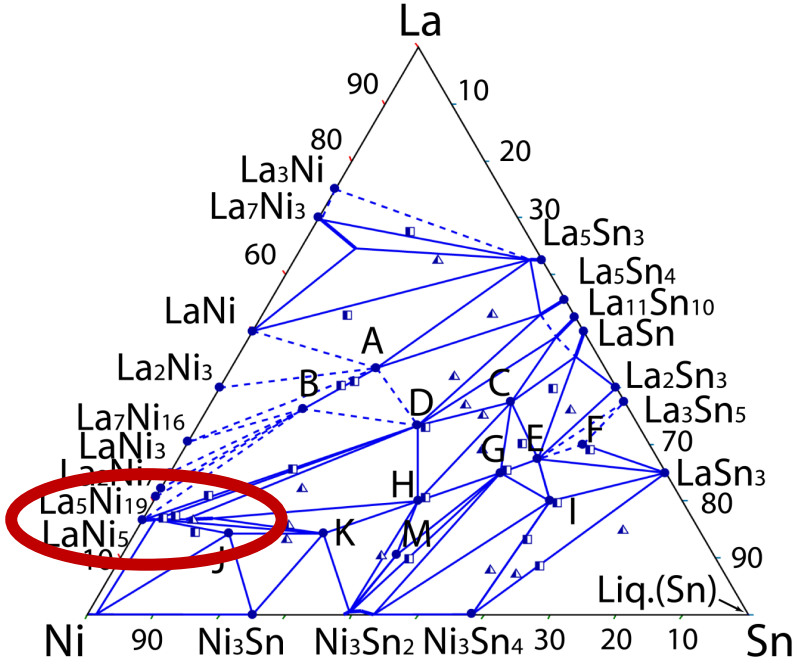
$LaSn_5$: hexagonal *P6/mmm* cell with all *3g* and *2c* sites occupied by Sn

Formation energy: -0.283 eV/atom

-0.107 eV/atom

$$E_{\text{formation}} = \frac{E(LaNi_5) - 1\cdot E(\text{hex La}) - 5\cdot E(\text{fcc Ni})}{6}$$

$$E_{\text{formation}} = \frac{E(LaSn_5) - 1\cdot E(\text{hex La}) - 5\cdot E(\alpha\text{-Sn})}{6}$$



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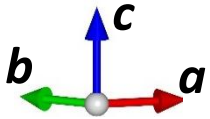
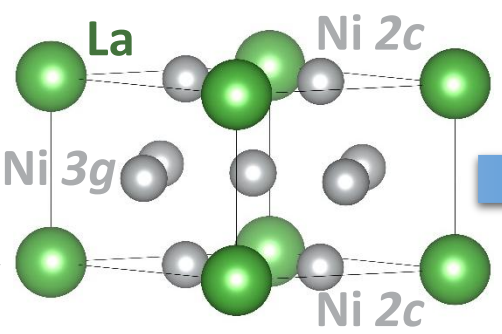
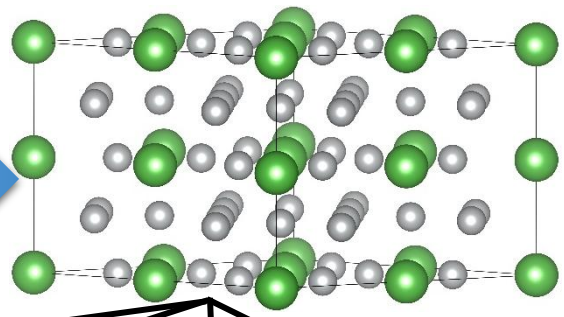




2x2x2 multiple



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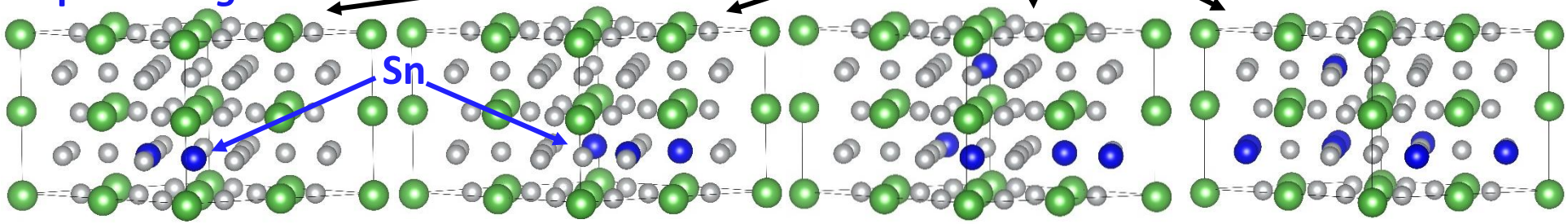

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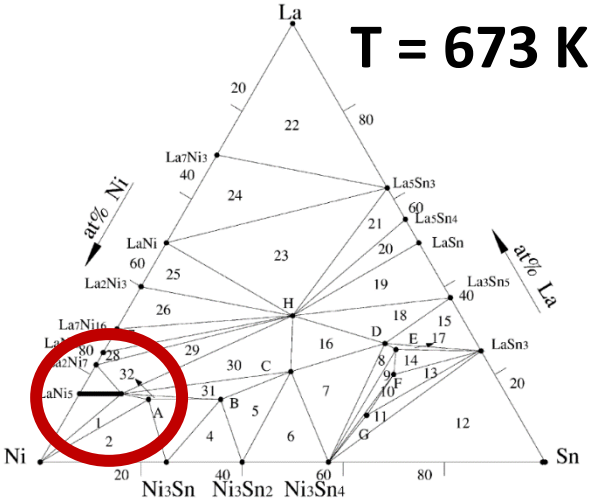

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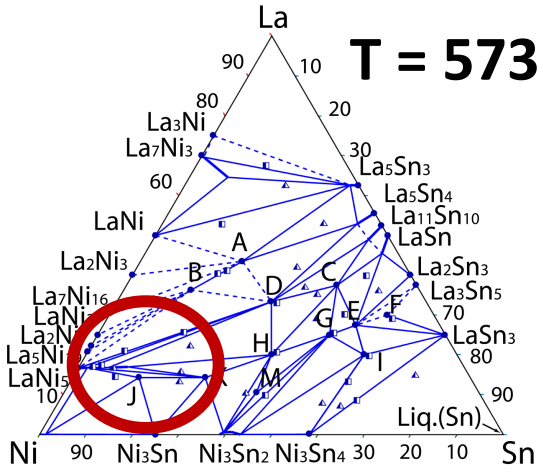

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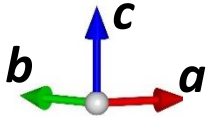

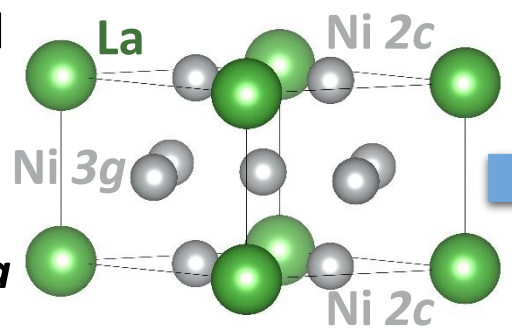

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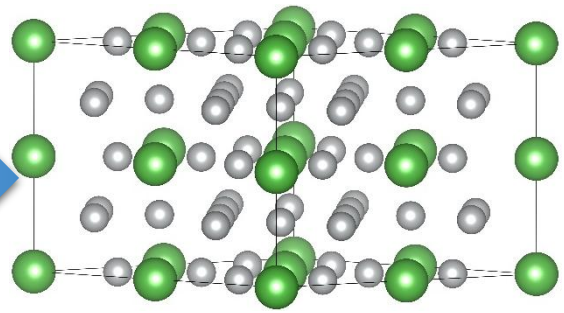

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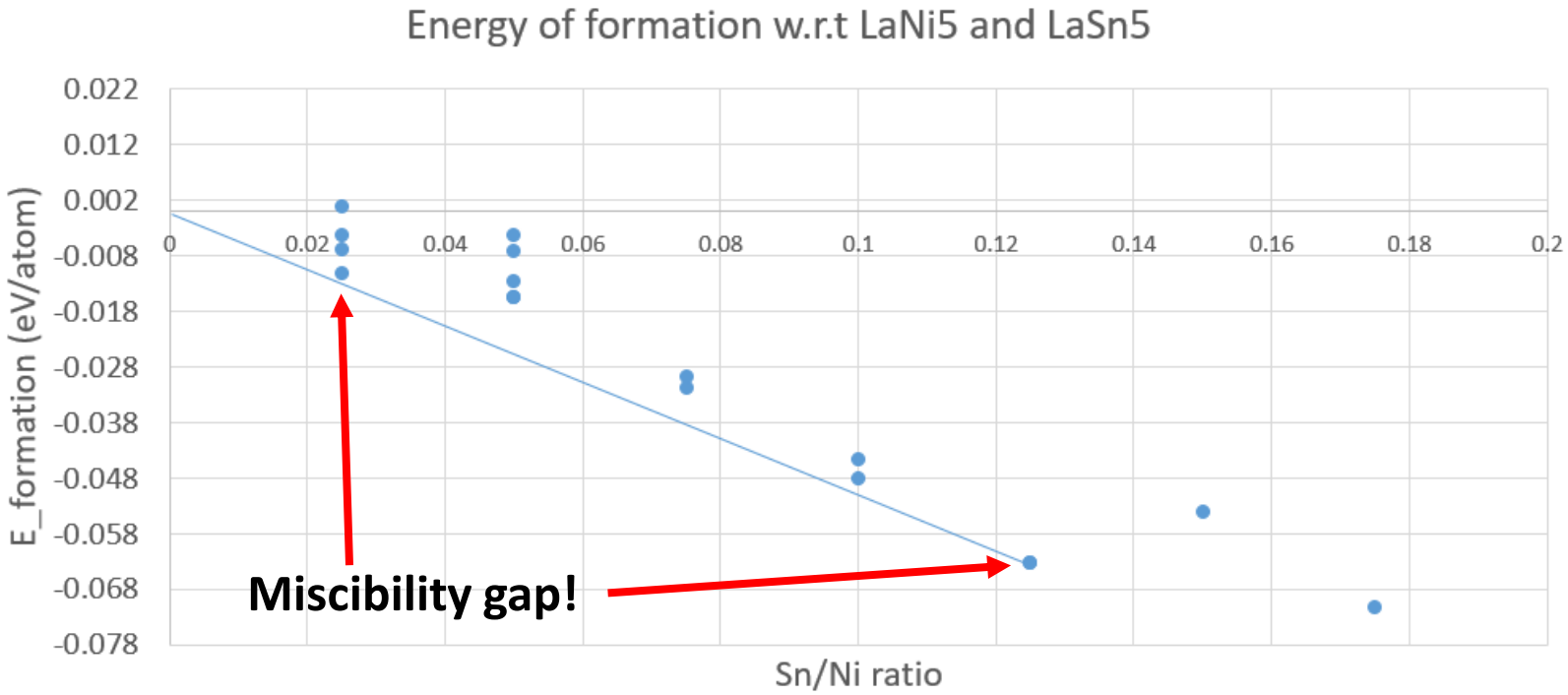

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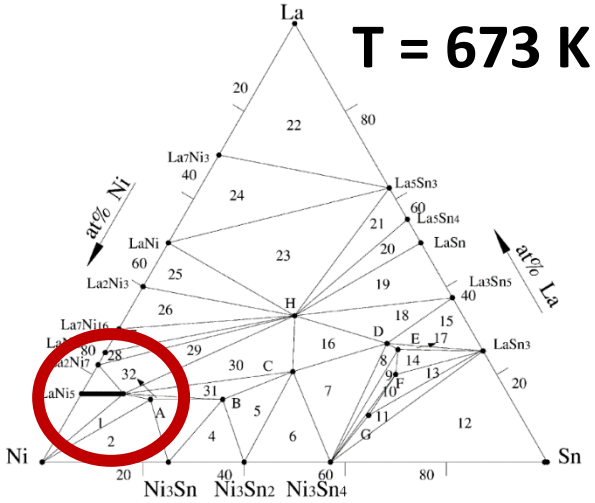

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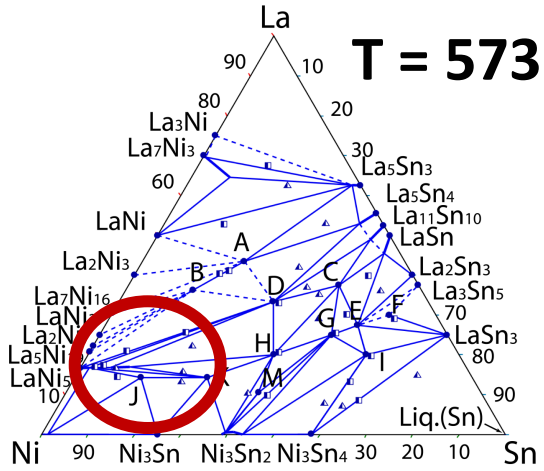

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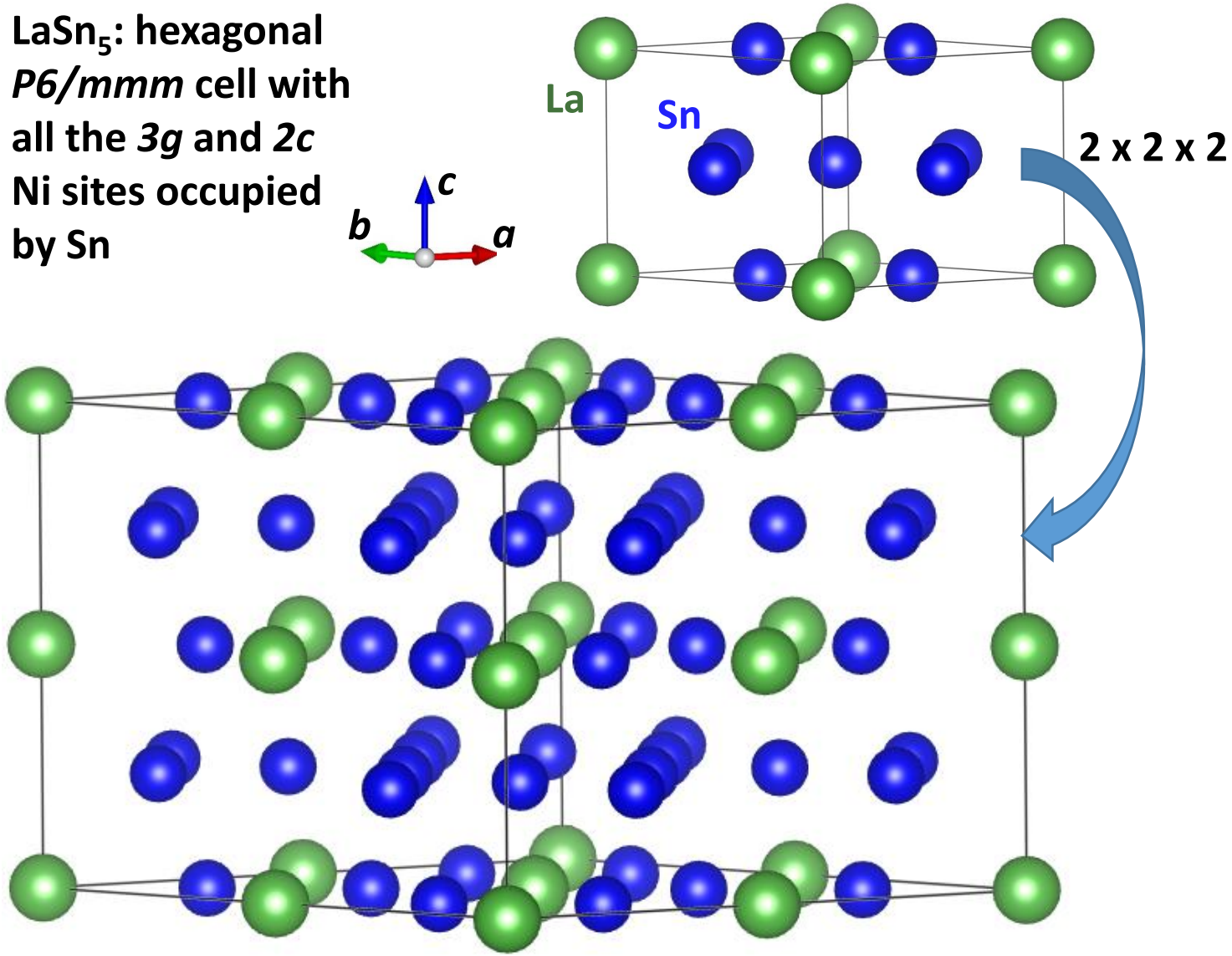
ipm

Phonons of $LaSn_5$

$LaSn_5$: hexagonal *P6/mmm* cell with all the *3g* and *2c* Ni sites occupied by Sn



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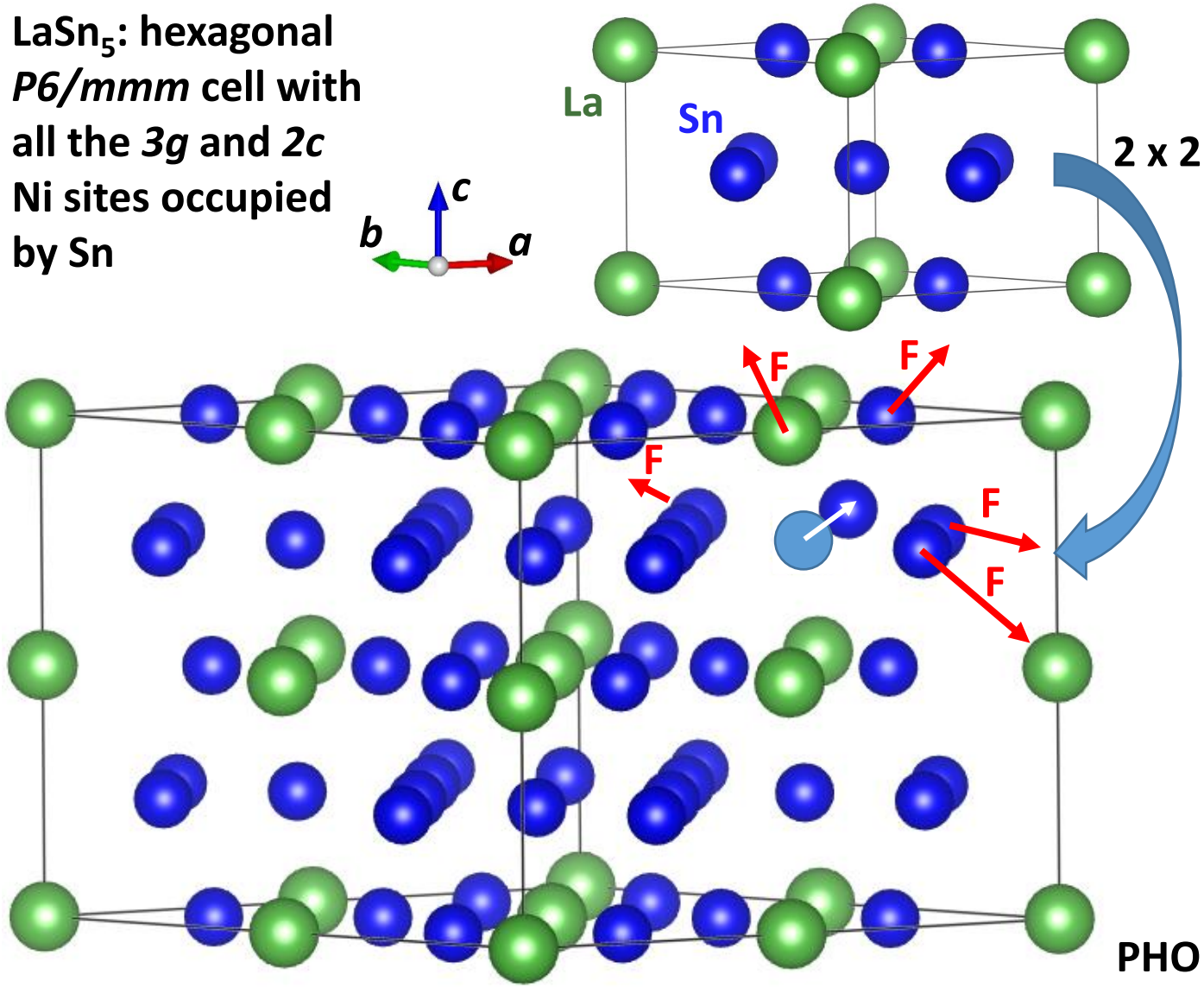

Displacement of every crystallographically non-equivalent atom along every crystallograpohically non-equivalent direction

PHONOPY software

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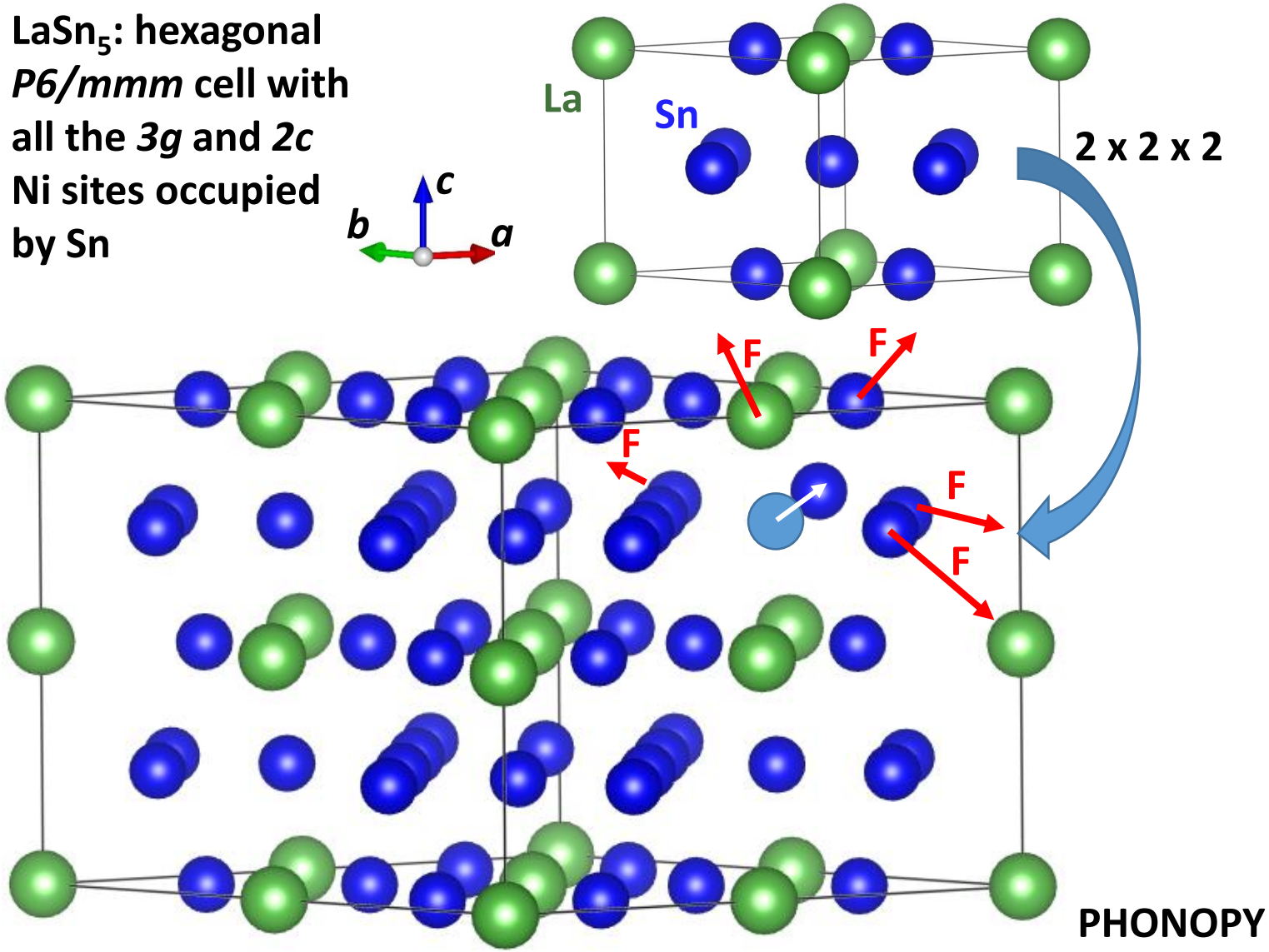

Helmholtz free energy *F*

$$F = \frac{1}{2}\sum_{\mathbf{q}\nu}\hbar\omega(\mathbf{q}\nu) + k_\mathrm{B}T\sum_{\mathbf{q}\nu}\ln[1-\exp(-\hbar\omega(\mathbf{q}\nu)/k_\mathrm{B}T)],$$

Phonon energy *E*

$$E = \frac{1}{2}\sum_{\mathbf{q}\nu}\hbar\omega(\mathbf{q}\nu) + \sum_{\mathbf{q}\nu}\hbar\omega(\mathbf{q}\nu)\frac{1}{\exp(\hbar\omega(\mathbf{q}\nu)/k_\mathrm{B}T)-1},$$

Entropy *S* and heat capacity C_v

$$S = -\left(\frac{\partial F}{\partial T}\right), \quad C_\mathrm{v} = -\left(\frac{\partial E}{\partial T}\right)_\mathrm{v}.$$

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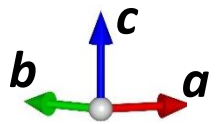

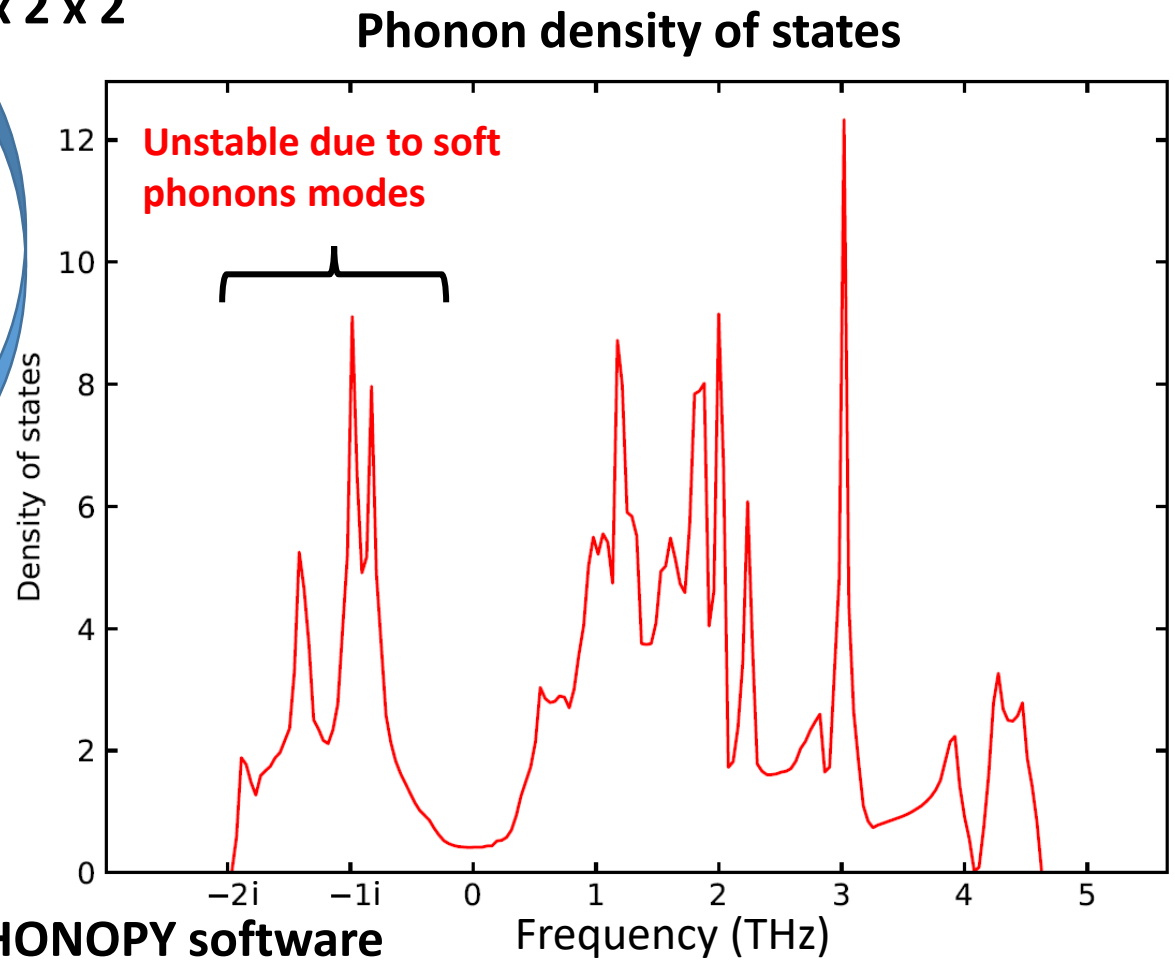

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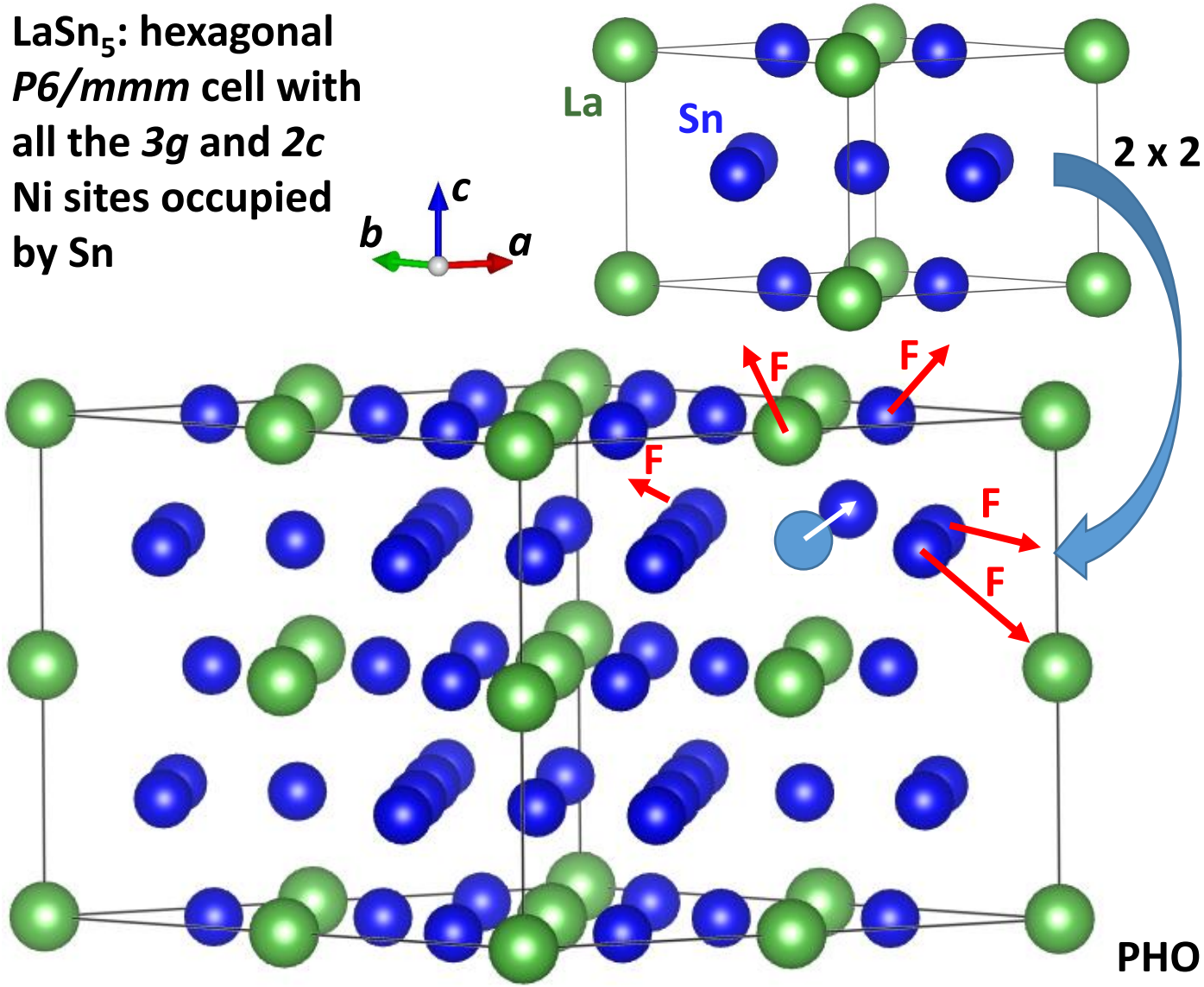

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Phonons in $La(Ni,Sn)_5$: *ab initio* study

MATUR

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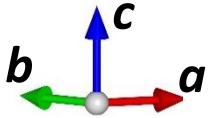

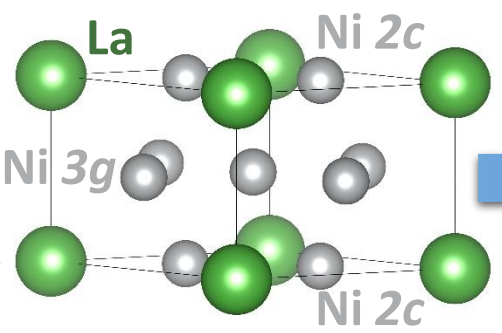

2x2x2 multiple

Sn atoms substituting Ni atoms are computed in 48-atom cell

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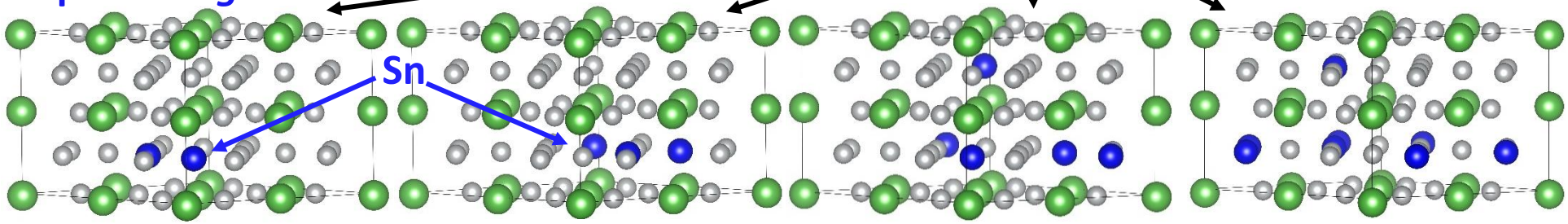
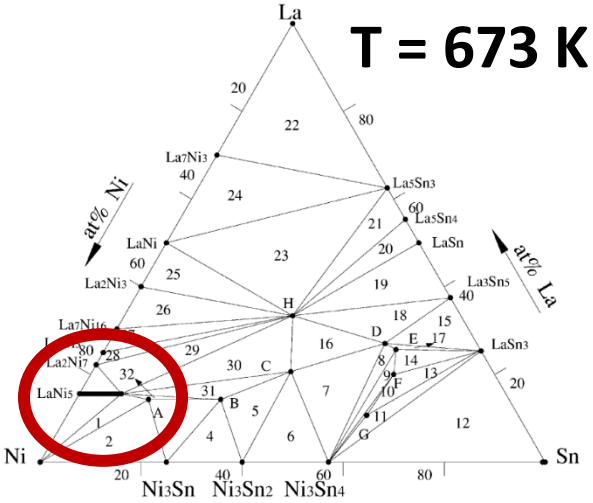
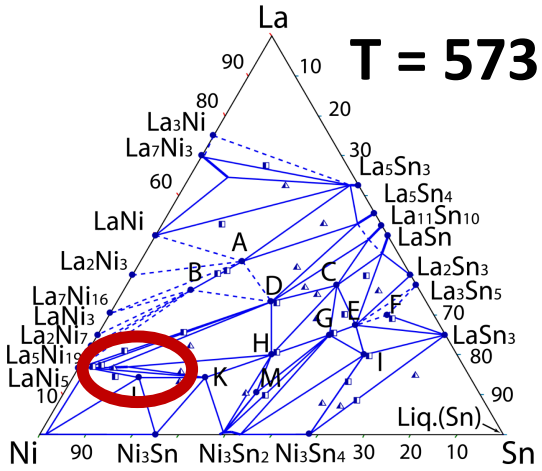


T = 673 K



Y. Zhuang *et al.*, J. of Alloys and Comps. 363 (2004) 228.

T = 573 K



O. Zobač *et al.*, *under review* DOI:10.2139/ssrn.5228280

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Phonons in $La(Ni,Sn)_5$: *ab initio* study

MATUR

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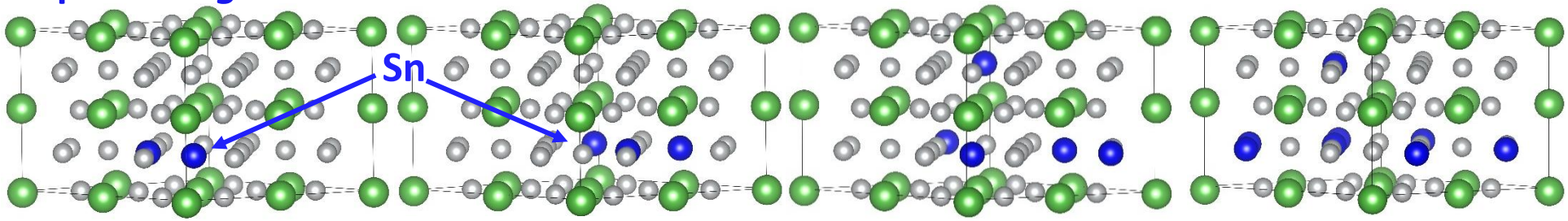

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LaNi5-3xSn-na-3g-SQS-48-atoms-NM-phonopy-DONE-no-imag

168 displacements
251 GB of disk space
Barbora 16 nodes
1000 – 2000 node hours

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Phonons in $La(Ni,Sn)_5$: *ab initio* study

MATUR

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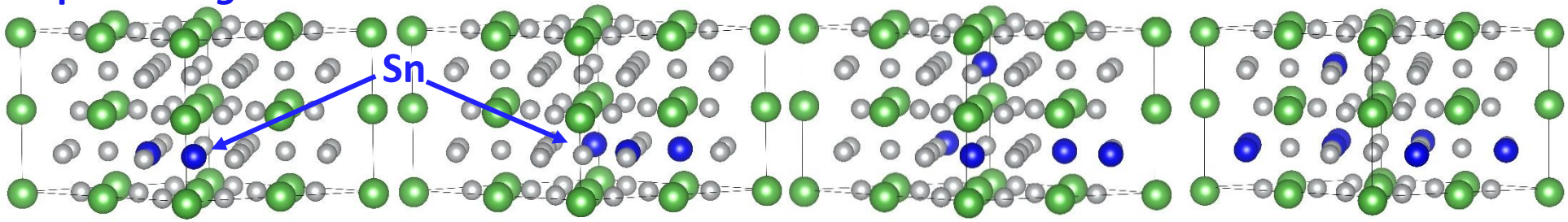

LaNi5-1xSn-na-2c-48-atoms-DONE-phonopy-DONE-no-imag

288 displacements

500 GB of disk space

Karolina 4 nodes

300 - 500 node hours

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Stability of $La(Ni,Sn)_5$: *ab initio* study

MATUR

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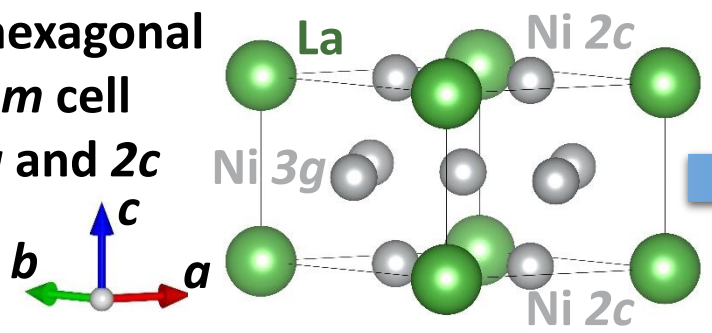

2x2x2 multiple

Sn atoms substituting Ni atoms are computed in 48-atom cell

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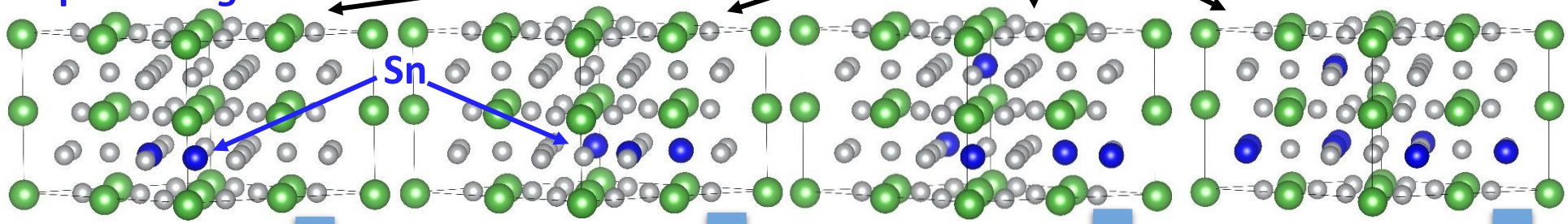
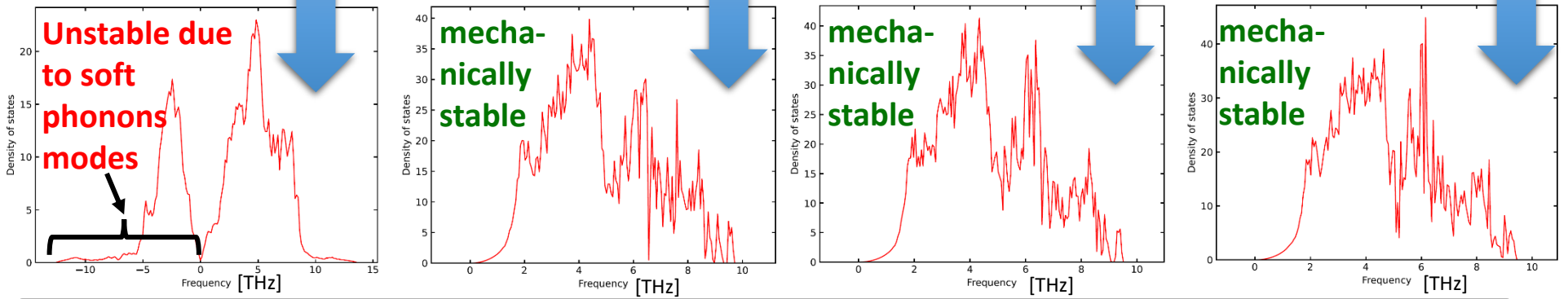
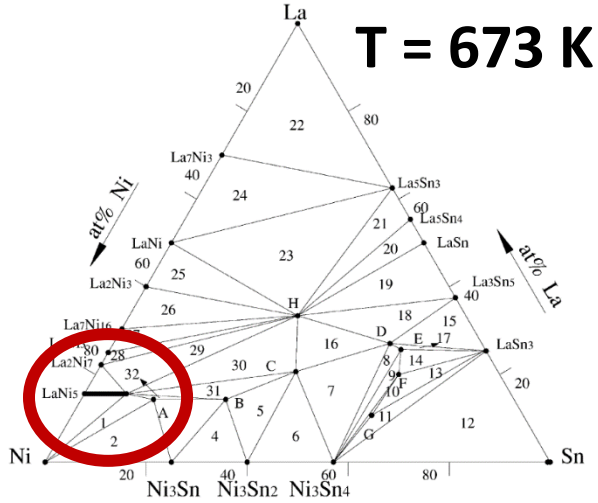
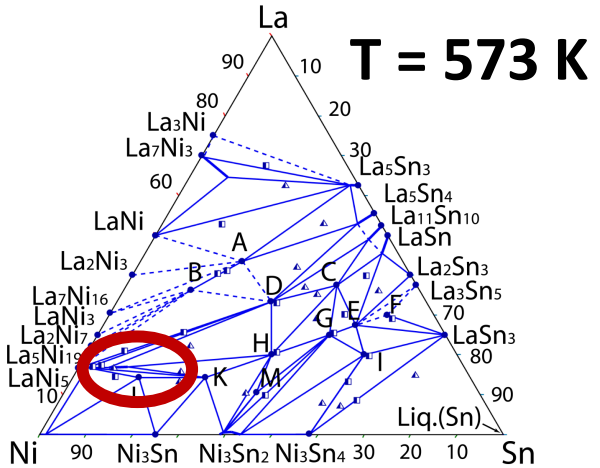




Phonon calculations of Sn-states: test of mechanical and thermodynamic stability.



Y. Zhuang *et al.*, J. of Alloys and Comps. 363 (2004) 228.



O. Zobač *et al.*, *under review* DOI:10.2139/ssrn.5228280

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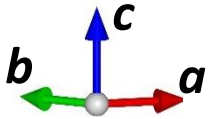

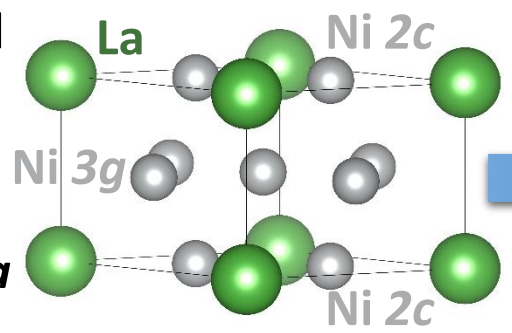

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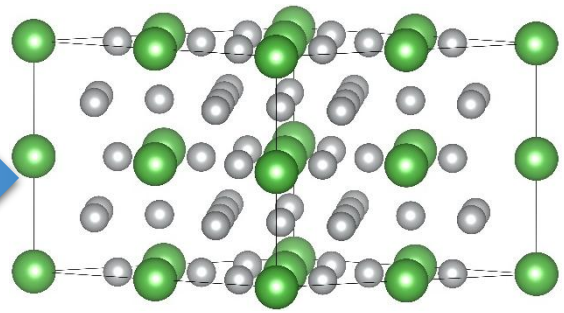

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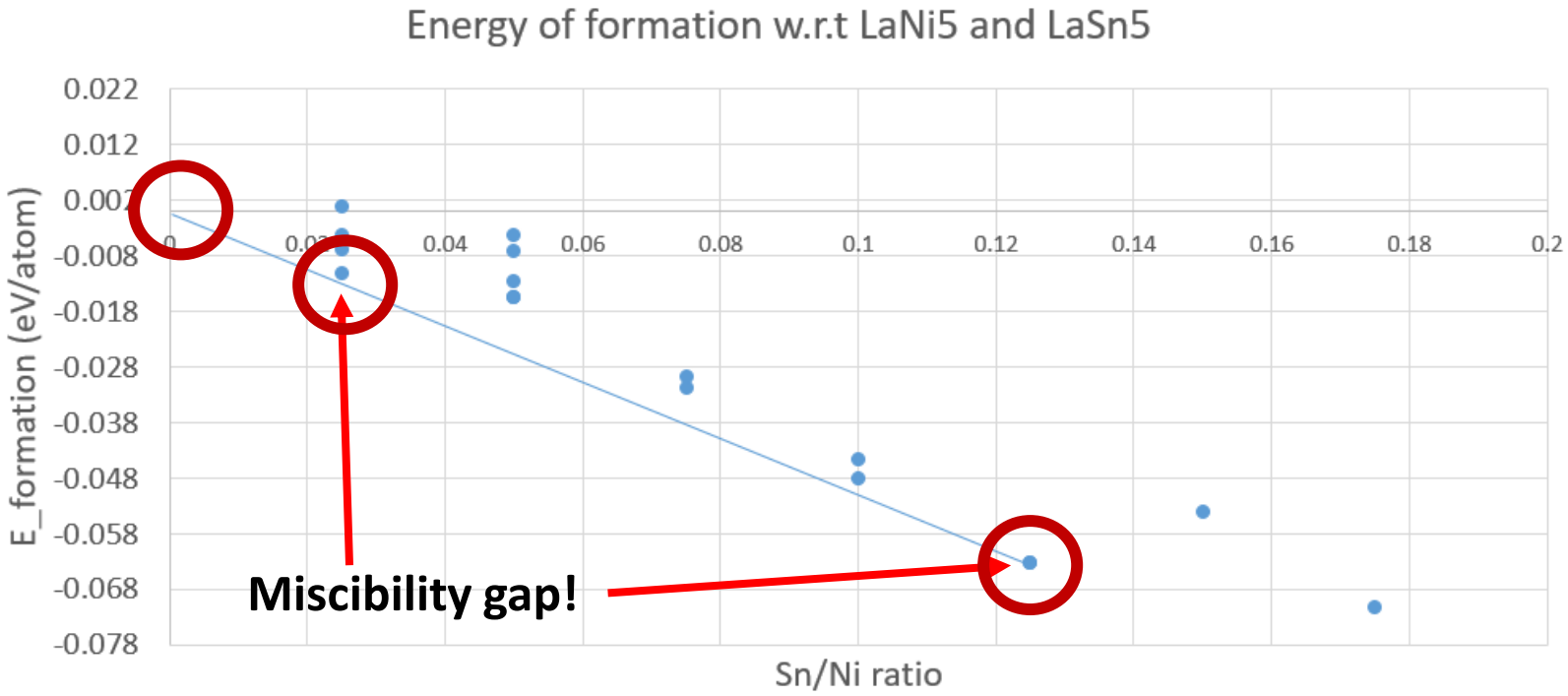

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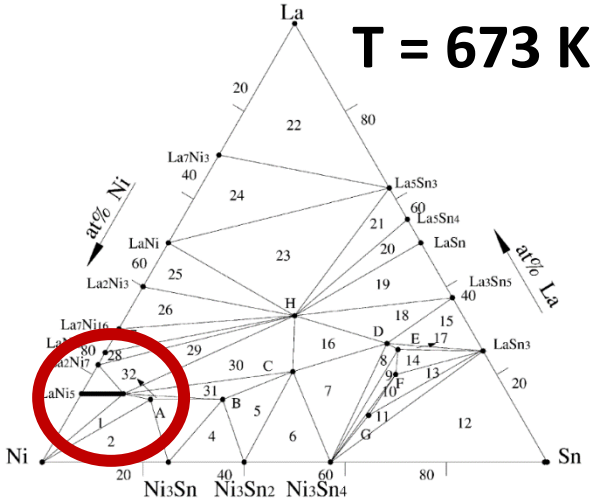

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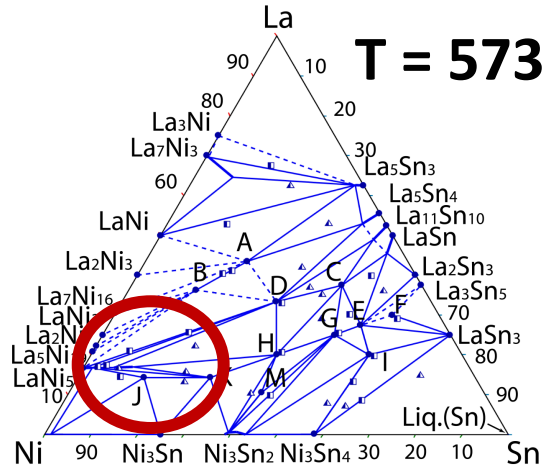

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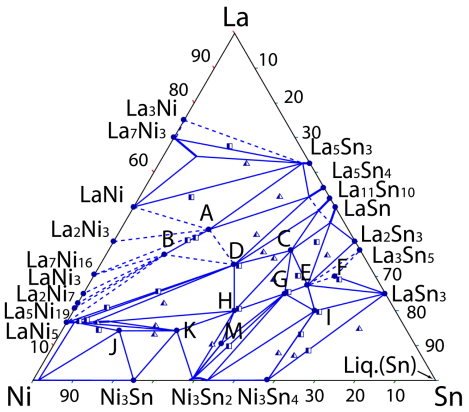
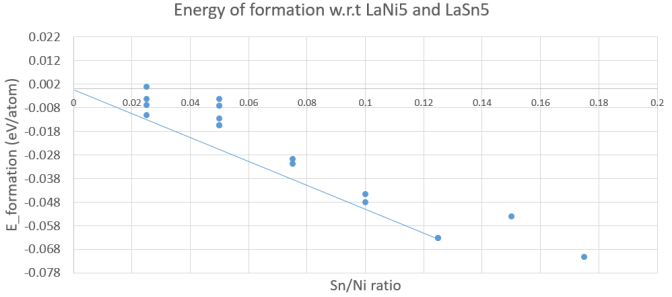
Conclusions

- Thermodynamics of H-storage La-Ni-Sn materials is complex.
- We focused on the **solubility of Sn in $LaNi_5$**.
- Our calculations confirm the existence of a miscibility gap.
- **Sn atoms destabilize $LaNi_5$** but in a non-trivial manner when **$LaSn_5$** is unstable both thermodynamically and mechanically (there are imaginary-frequency „soft“ phonon modes) but miscibility-gap end-members are stable.





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Thank you for your attention!

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