

## Curriculum Vitae of Leyla Isaeva

### Work experience:

**December 2015-till now:** PostDoc, Condensed matter division, SISSA, Trieste, Italy

### Education:

**2010-2015:** PhD student, Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden. 2015: PhD thesis entitled “Amorphous and crystalline functional materials from first principles”.

**2004-2010:** MS in physics, *Summa cum laude*, M.V.Lomonosov Moscow State University, Department of Physics, Solid State Physics Division, Moscow, Russia

**2000-2004:** School No. 57, mathematical class, Moscow, Russia

**1994-2000:** School No. 1253, Moscow, Russia

### Languages

Russian (native), English (fluent), Italian (intermediate), Swedish (beginner), Azerbaijani

### Skills

1. Programming languages: Fortran, Python, bash.
2. Matlab, Mathematica
3. VASP, Quantum ESPRESSO, LAMMPS; post processing tools as XCrySDen, Vesta, VMD, Gnuplot, Matplotlib.
4. SSH client user.

### Research Interests

1. Heat transport in disordered systems
2. Phase transitions;
3. *Ab initio* Total Energy, and Phonon Calculations for solid states;
4. Hydrogen Storage Materials;
5. Shape memory alloys;
6. Martensitic transitions and collective phenomena.

### Awards

**December, 2009:** Honored Diploma, III International Symposium on Hydrogen Energetics, Moscow;

**December, 2008:** Russian Federation President Scholarship for Outstanding Young People;

**May, 2008:** 1<sup>st</sup> place in Scientific Research Competition “Lomonosov-2008”;

**May, 2006:** 1<sup>st</sup> place in Scientific Research Competition in physics between second year students of Moscow State University;

**2000-2004:** Diplomas in Physics, Mathematics, and Psychology of different Olympiads for pupils.

### Conferences

### **Tutorials:**

**Jan 2017:** *Advanced Workshop on High-Performance & High-Throughput Materials Simulations using Quantum ESPRESSO, Hands-on session DFPT and Phonon calculations, ICTP, Trieste*

I have written an interface between Quantum ESPRESSO and my own Python3 code which allows finite difference phonon spectra calculations; I have also prepared a presentation which reviews the method for the participants of the workshop, prepared exercises, helped them to run and understand the codes and the exercises.

### **Talks:**

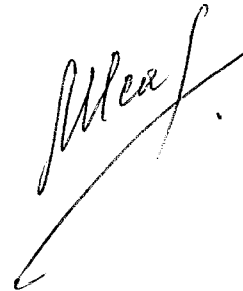
1. *"First principles lattice dynamics of the martensitic transition in AuZn"*, Balatonfured, Hungary April 2013, Invited talk.
2. *"Phonon instabilities in cubic AuZn"*, L.Isaeva, P.Souvatzis, O.Eriksson, Turku, Finland February 2012, Invited talk
3. *"Crystal phases of FeS<sub>2</sub>"*, Challenges within electronic structure theory and its applications for materials modeling, Department of Physics, Chemistry and Biology (IFM), Linkoping University, Linkoping, Sweden, March 2009;
4. *"Study of dynamical stability of the defect phase of palladium hydride"*, Isaeva L., Bazhanov D., Isaev E., Ereemeev S., Kulkova S., Abrikosov I., III International Symposium on Hydrogen Energetics, Moscow, Russia, December 1-2 2009, Moscow, Russia;
5. *"Dynamical stability of palladium hydride: ab initio study"*, Isaeva L.E., Bazhanov D.I., Isaev E.I., Ereemeev S.V., Kulkova S.E., Abrikosov I.A., International Conference on Hydrogen Materials Science and Chemistry of Carbon Nanomaterials" ICHMS'2009, Yalta, Crimea, Ukraine, August 25-31 2009;
6. *"Interaction of vacancy and hydrogen-vacancy complex with 3d-transition metal impurities in palladium crystal"*, The Sixth National Conference on Application of X-Ray, Synchrotron Radiation, Neutrons and Electrons for Material Characterization, Shubnikov Institute of Crystallography RAS, Moscow, Russia, November 2007;

### **Posters:**

1. *"Influence of magnetism on interaction energy between 3d impurities and hydrogen in palladium crystal in the presence of vacancies"*, Moscow International Symposium on Magnetism, M.V.Lomonosov Moscow State University, Moscow, Russia, June 20-25, 2008;
2. *"Dynamical stability of the defect phase of palladium hydride: ab initio study"*, Fifth International Alloy Conference (IAC-V), Ruedgen, Germany, September 11-14, 2008;
3. *"First principle study of the dynamical stability of the defect phase of palladium hydride"*, Functional nanomaterials and high-purity matters, Suzdal, Russia, September 29 – October 3, 2008;
4. *"Dynamical stability of the defect phase of palladium hydride: ab initio study"*, Multilevel approaches in physical mesomechanics. Fundamental aspects and engineering applications, Tomsk, Russia, September 9-12, 2008;
5. *"Dynamical stability of the defect phase of palladium hydride: ab initio study"*, The CAMD Summer School, Lyngby, Denmark, August 17-19, 2008;
6. *"First principles studies of anomalies in phonon spectra of Heusler alloys"*, National Conference on Application of X-Ray, Synchrotron Radiation, Neutrons and Electrons for Material Characterization,

Nano-Bio-Info-Cognitive Technologies, Shubnikov Institute of Crystallography RAS, Moscow, Russia, November 16-21, 2009.

7. "Dynamic stabilization of cubic AuZn", 14th International Conference on Martensitic Transformations (ICOMAT), Bilbao, Spain, July 2014

A handwritten signature in black ink, appearing to read "M. Kozlov", written in a cursive style. The signature is positioned on the right side of the page.

