

Petros Souvatzis

Curriculum Vitae

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Education

- 2007 **Doctor of Philosophy**, *Uppsala University*, Uppsala.
Subject: Physics
- 2001 **Master of Science**, *Uppsala University*, Uppsala.
Main subject: Physics
- 1999 **Master of Education for the Upper Secondary School**, *Uppsala University*, Uppsala, Subjects: Physics and Mathematics.

Phd thesis

title *Electronic Structure and Lattice Dynamics of Elements and Compounds*
supervisor Prof. Olle Eriksson
download at: <http://publications.uu.se/abstract.xsql?dbid=8198>

Master thesis

title *The Linearized Theory of Gravitational Radiation, and the Detection of Gravitational Waves*
supervisor Prof. Ulf Danielson
download at: <http://www.teorfys.uu.se/courses/exjobb/>

Developed open access computer programs

- I. The code `scph`, developed by Petros Souvatzis, in which the Self Consistent Ab Initio Lattice Dynamical method (SCAILD) has been implemented. The code and corresponding manual can be found at:

<http://www.uquantchem.com/scaild.html>

- II. The `uquantchem` code (Uppsala Quantum Chemistry package) is a program developed by P. Souvatzis. The code is designed to solve the non-relativistic Schrödinger equation for atoms and molecules using gaussian basis sets. Amongst the capabilities are:

- (1) Unrestricted Hartree Fock (URHF)
- (2) Restricted Hartree Fock (RHF)
- (3) Configuration Interaction calculations including Singles and Doubles (CISD)
- (4) Møller-Plesset manybody perturbation calculations to 2:nd order (MP2)
- (5) Diffusion Quantum Monte Carlo (DQMC)
- (6) Variational Quantum Monte Carlo (VMC)

- (7) Density Functional Theory (DFT) calculations
- (8) Time Dependent Density Functional Theory (TDDFT) calculations
- (9) Extended Lagrangian Born-Oppenheimer Molecular Dynamics (XL-BOMD)
- (10) Fast First Principles Molecular Dynamics (FFP-MD)
- (11) OPENMP and MPI parallelization

The code and corresponding manual can be found at:

<http://www.uquantchem.com/uquantchem.html>

Work experience

- 2014- **Computational Physicist**, *EQUA-Simulation AB*.
- 2010-2014 **Lecturer**, *Uppsala University*, Computational Physics. 1FA573
- 2010-2014 **Lecturer**, *Uppsala University*, Foundations of physics teaching. 1FA520
- 2010-2014 **Researcher**, *Uppsala University*, Uppsala, Sweden.
- 2011-2014 **PhD Student Supervisor**, *Uppsala University*.
Supervisor for Leyla Isaeva
- 2012-2013 **Administration**, *Worked as an applications expert on the Uppmax computer cluster* .
- 2010 **Post doc**, *Royal Institute of Technology (KTH)*, Stockholm, Sweden.
- 2008-2009 **Post doc**, *Los Alamos National Laboratory*, Los Alamos, New Mexico USA.
- 2007 **Physics Teacher** , *Uppsala University*, Uppsala.
Teacher in Analytical mechanics (Civil engineering program).
- 2002-2007 **Phd Student**, *Uppsala University*, Uppsala.
- 2004 **Master Thesis Supervisor**, *Uppsala University*, Uppsala.
Supervisor for Computer Science student Angela Sjöholm
Title of thesis:
Development of User Interface for Simulation Program of Material Calculations
- 2001-2002 **Physics and Mathematics Teacher**, *Fyrisskolan*, Uppsala.
Students aged 16-20 yr
- 1999-2001 **Physics and Mathematics Teacher**, *Celciusskolan*, Uppsala.
Students aged 16-20 yr

Programming skills:

- (1) **Languages**, Fortran, C++, Python, Matlab.
- (2) **Editors/debuggers**, Windows Visual Studio, gdb, Valgrind.
- (3) **Script-languages**, Perl, bash, tcsh.
- (4) **Operating-systems**, UNIX, Windows.
- (5) **Parallel computing protocols**, MPI, OPENMP.
- (6) **Web**, html, SQL.

Languages

Swedish	native
English	fluent
Greek	good
French	good

List of publications

- I. *Surface energies and work functions of the transition metal carbides*,
H. W. Hugosson, O. Eriksson, U. Jansson, A. V. Ruban, P. Souvatzis and I. A. Abrikosov, Surf. Sc. **557**, 243-254 (2004)
- II. *Elastic properties of $Mg_{1-x}Al_xB_2$ from first principles theory*,
P. Souvatzis, J. M. Osorio-Guillén, R. Ahuja, A. Grechnev, O. Eriksson, J.Phys.:Condens. Matter, **16**, 5241 (2004)
- III. *First-principles prediction of superplastic transition-metal alloys*,
P. Souvatzis, M. I. Katsnelson, S. Simak, R. Ahuja, O. Eriksson and P. Mohn, Phys. Rev. B **70**, 012201 (2004)
- IV. *Calculation of the equation of state of fcc Au from first principles*,
P. Souvatzis, A. Delin, O. Eriksson, Phys. Rev. B **73**, 054110 (2006)
- V. *Anomalous thermal expansion in α -titanium*,
P. Souvatzis O. Eriksson, M. I. Katsnelson, Phys. Rev. Lett. **99**, 015901 (2007)
- VI. *Entropy driven stabilization of energetically unstable crystal structures explained from first principles theory*.
P. Souvatzis, O. Eriksson, M. I. Katsnelson and S. P. Rudin,
Phys. Rev Lett. **100**, 095901 (2008)
- VII. *Ab-initio calculations of the phonon spectrum and the thermal expansion for the 4d metals*, P. Souvatzis and O. Eriksson, Phys. Rev. B **77**, 024110 (2008)
- VIII. *Elasticity of the superconducting metals V, Nb, Ta, Mo and W at high pressure*,
L. Koči, Y. Ma, A. Oganov, P. Souvatzis and R. Ahuja,
Phys. Rev. B **77**, 214101 (2008)
- IX. *The self consistent ab-initio lattice dynamical method*.
P. Souvatzis, O. Eriksson, M.I. Katsnelson and S. P. Rudin, Comput. Mater. Sci. **44**, 888-894 (2009)
- X. *Dynamical stabilization of cubic ZrO_2 by phonon-phonon interactions: Ab initio calculations*,
P. Souvatzis and S. P. Rudin, Phys. Rev. B **78**, 184304 (2008)

- XI. *Dynamical stabilization of the body centered cubic phase in lanthanum and thorium by phonon-phonon interaction*
P. Souvatzis, T. Björkman, O. Eriksson, P. Andersson, M. I. Katsnelson and S. P. Rudin, *J.Phys.:Condens. Matter*, **21**, 175402 (2009)
- XII. *Ab initio study of interacting lattice vibrations and stabilization of the β -phase in Ni-Ti shape-memory alloy* P. Souvatzis, Dominik Legut, Olle Eriksson and M. I. Katsnelson, *Phys. Rev. B* **81**, 092201 (2010)
- XIII. *Dynamical stability of body center cubic iron at the Earths core conditions*
W. Luo, B. Johansson, O. Eriksson, S. Arpan, P. Souvatzis, M. I. Katsnelson and R. Ahuja, *PNAS* **107**, 9962-9964 (2010)
- XIV. *Density functional study of electronic structure and lattice dynamics of SrCl₂*
K. V. Krishnan, S. V. Ganapath, P. Souvatzis, O. Eriksson, S. Lebegue, *J.Phys.:Condens. Matter*, **22**, 445402 (2010)
- XV. *Entropically Stabilized Local Dipole Formation in Lead Chalcogenides*
Emil S. Božin, Christos D. Malliakas, Petros Souvatzis, Thomas Proffen, Nicola A. Spaldin, Mercuri G. Kanatzidis, and Simon J. L. Billinge, *Science*, **330** 1660-1663,(2010)
- XVI. *Ab initio Elasticity model for the evaluation of structural parameters in multilayer systems with applications to transition metal and Si-based multilayers*
Mikael Råsander, Petros Souvatzis, Anders Höglund, and Olle Eriksson, *Phys. Rev. B* **84**, 125424 (2011)
- XVII. *Phonon lifetimes from first-principles self-consistent lattice dynamics*
Petros Souvatzis, *J.Phys.:Condens. Matter* **23**, 445401 (2011)
- XVIII. *Temperature-driven α -to- β phase transformation in Ti, Zr and Hf from first-principles theory combined with lattice dynamics* P. Souvatzis, S. Arapan, Olle Eriksson and M. I. Katsnelson, *Europhys. Lett. B* **96**, 6606 (2011)
- XIX. *High-temperature phonon stabilization of γ -uranium from relativistic first-principles theory* P. Söderlind, B. Grabowski, L. Yang, A. Landa, T. Björkman, P. Souvatzis and Olle Eriksson. *Phys. Rev. B* **85**, 060301(R) (2012)
- XX. *Extended Lagrangian Born-Oppenheimer molecular dynamics in the limit of vanishing self-consistent field optimization.* P. Souvatzis. and A. M.N Niklasson, *J. Chem. Phys.*, **139**, 214102 (2013)
- XXI. *Uquantchem: A versatile and easy to use Quantum Chemistry Computational Software.* P. Souvatzis. *Comp. Phys. Comm.* **185**, 415-421 (2014)

- XXII. *First principles molecular dynamics without self-consistent field optimization.*
P. Souvatzis. and A. M.N Niklasson, J. Chem. Phys., **140**, 044117 (2014)
- XXIII. *Lattice dynamics of cubic AuZn from first principles.*
L. Isaeva, P. Souvatzis., O. Eriksson and J. C. Lashley, Phys. Rev. B **89**, 104101 (2014)
- XXIV. *Interplay between effect of Mo and chemical disorder on the stability of β/β_o -TiAl phase*
David Holec, Domink Legut, Leyla Isaeva, Petros Souvatzis, Helmut Clemens, Svea Mayer , Intermetallics **61**, 85-90 (2015)
- XXV. *Lattice Dynamics and Chemical Bonding in Sb_2Te_3 from first principles calculations*
Bao-Tian Wang, Petros Souvatzis, Olle Eriksson, and Ping Zhang, J. Chem. Phys., **142**, 174702 (2015)

List of Invited talks

- I. The Abus Salam International Centre for Theoretical Physics, Trieste, Italy. The 15:th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, 13-15 January 2011, presenting: Self-consistent ab-initio lattice dynamics (SCAILD); theory and numerical examples.
- II. Centre de Physique Theorique, Ecole Polytechnique, Palaiseau, France, 2008 presenting: *Self-consistent phonon calculations from first principles*
- III. Université Henri Poincarè, Nancy, France, 2008 presenting:
Entropy driven stabilization of energetically unstable crystal structures explained from first principles
- IV. Uppsala University, Sweden, 2007, invited to the conferece: Frontiers of theoretical magnetism, presenting: *Self-consistent phonon calculations from first principles*
- V. Los Alamos National laboratory, New Mexico, USA, 2006, presenting:
Calculation of the equation of state of fcc Au from first principles
- VI. Prague, Czech Republic, 2006, invited to the conferece: Frontiers of theoretical magnetism, presenting: *Calculation of the equation of state of fcc Au from first principles*

List of talks

- I. MRS fall meeting in Boston, USA, 2007, Symposium E, presenting:
Entropy driven stabilization of energetically unstable crystal structures explained from first principles
- II. Psi-k conference in Berlin, Germany, 2010, Symposium on Vibrational Coupling, presenting: *Self-consistent phonon calculations from first principles*