

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

- 2017- **Senior Business Intelligence Developer**, *Etraveli*.
Development of algorithms for optimal pricing. The models are parameterized through statistical analysis of large sets of data. Typical methods are (1) simple regression (2) basis-set expansion of discrete data to enable utilization of conjugated gradient methods (3) ensemble learning to achieve revenue estimates. Apart from the mathematical tools SQL is used for querying the data, python is used for the non-computational intensive data handling whereas the more computationally intensive algorithms are written in FORTRAN and interfaced with python through wrappers utilizing f2py. For the regression ScikitLearn is used and the presentation of data is made through Qlikview and/or Jupyter notebooks
- 2014-2017 **Computational Physicist**, *EQUA-Simulation AB*.
Development of indoor climate simulation models. Programming in C++ and modelica. Focus was on optimizing the speed and stability of the control-algorithms in use.
- 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.
- (7) **Version handling**, GIT, Tortoise SVN .

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. Kočí, 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 ZrO₂ 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, Mercouri 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 Råsaender, 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*