Petros Souvatzis

Curriculum Vitae

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75237 Uppsala, Sweden
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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) **Script-languages**, Perl, bash, tcsh.
(3) **Operating-systems**, UNIX, Windows.
(4) **Parallel computing protocols**, MPI, OPENMP.
(5) **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 $SrCl_2$*

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 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. Universitè 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*