0.0.1 Report on the Psi-k/CECAM Event on Self-Interaction Correction: State of the Art and New Directions

September 18, 2011 (evening) to September 21, 2011

Ramada Jarvis Hotel, Chester, UK

Organisers:
Martin Lueders, Leon Petit and Zdzislawa (Dzidka) Szotek (STFC Daresbury Laboratory, UK)

Local administration:
Wendy Cotterill and Shirley Miller (STFC Daresbury Laboratory, UK)

Sponsored by
ESF/Charity Psi-k Network and CECAM Node at STFC Daresbury Laboratory (UK)

Webpage

`http://www.cse.scitech.ac.uk/cecam_at_daresbury/self-interaction_correction.shtml`

Scientific report

This Psi-k/CECAM event on "Self-Interaction Correction: state of the art and new directions" took place on the thirtieth anniversary of John Perdew and Alex Zunger's seminal paper on correcting self-interaction error inherent in local density approximation to density functional theory [Phys. Rev. B23, 5048 (1981)]. This paper had initiated a variety of new implementations, generalizations, and extensions of the proposed self-interaction correction (SIC) approach, nominally giving rise to a new "field". It had also led to a plethora of applications in different fields of physics and chemistry. Over the years, it had become apparent that different "varieties" of SIC had been developed nearly independently of each other, in particular in the field of quantum chemistry and solid state physics, with the experiences/advances gained in one field barely

noticed in the other areas. Thus the paramount goal of this event was to bring together, for the first time, all the groups that had applied and worked on self-interaction correction, in order to discuss and assess the state of the art of all the different flavours of SIC, share the experiences and identify the most important and burning issues, unsolved problems, and perhaps find a common direction for future developments.

The meeting took place in a beautiful city of Chester, the capital of the Cheshire county, U.K. The city is unique in its rich history, and comfortably ranks alongside the cities of London, York, Bath and Edinburgh. Chester was founded by the Romans over 2000 years ago, and much of the Roman influence remains and Chester City Walls are the most complete in Britain. The venue of the meeting, the Ramada Chester Hotel, is situated 2 miles away from the centre of the city, in a quiet, green area. It provided nice and enjoyable atmosphere for the lectures and lively discussions.

The event attracted over 40 participants from all over the world, with 11 from the U. K., the country of the organizers of the meeting, seven from the USA, six from Germany, three each from Denmark and Iceland, two from France, Italy, Ireland, Japan, and Switzerland, and one from Brazil and Sweden. It was organized around 20 invited talks of 45 minutes (see the list below), a poster session to allow participants to present and discuss their contributed papers, and a two-hours long, concluding and summarizing, round table discussion.

Invited Speakers

Hisazumi Akai (Osaka University, Japan)
Björn Baumeier (MPI Mainz, Germany)
Klaus Capelle (Sao Paulo, Brazil)
Aron Cohen (Cambridge, UK)
Olle Eriksson (Uppsala University, Sweden)
Alessio Filippetti (Cagliari, Italy)
Nikitas Gidopoulos (STFC RAL, U.K.)
Peter Küepfel (Faculty of Science, VR-II, Univ. of Iceland)
Stephan Kuemmel (University of Bayreuth, Germany)
Nicola Marzari (University of Oxford, UK)
Mark R. Pederson (NRL,USA)
John P. Perdew (Tulane University, USA)
Adrienn Ruzsinszky (Tulane University, USA)
Stefano Sanvito (Trinity College Dublin, Ireland)
Thomas C. Schulthess (ETH Zurich, Switzerland)
Julie B. Staunton (Warwick University, UK)
Eric Suraud (University of Toulouse, France)
Axel Svane (Aarhus University, Denmark)
Takao Tsuneda (Yamanshi University, Japan)
Alex Zunger (Colorado University Boulder, USA)

Moderator of Round Table Discussion:

George Malcolm Stocks (ORNL, USA)

Poster Session Presentations: Chair: Antonios Gonis (LLNL)

Markus Daene (Oak Ridge)
"Computationally Simple, Analytic, Closed Form Solution of the Self-Interaction Problem in Kohn-Sham Density Functional Theory"

Guntram Fischer (Halle)
"Magnetic Properties of Polar ZnO Surfaces: Application of SIC"

Hildur Guðmundsdóttir (Reykjavik)
"Self-interaction correction within the PAW formalism: implementation and applications"

Dirk Hofmann (Bayreuth)
"Self-interaction correction in the time-dependent Kohn-Sham scheme"

Simon Klüpfel (Reykjavik)
"More complex than expected: The Self-interaction corrected ground state of atoms and molecules"

Martin Lueders (Daresbury)
"Flavours of SIC"

Keld Lundgaard (Lyngby)
"Exchange correlation functionals including non-local correlation and error estimation"

The meeting was officially opened on Monday morning by Walter Temmerman, representing both the Psi-k ESF/Charity and the Daresbury node of CECAM, the institutions sponsoring the event. The opening invited talk of the meeting was by John Perdew, presenting his thoughts on SIC after 30 years. He discussed the dramatic successes and failures of the original Perdew and Zunger (PZ) SIC formulation. He also proposed two variants of PZ-SIC thus providing useful foundation for the rest of the meeting. Alex Zunger followed with his invited talk, addressing issues of the violation of the linear behaviour of the total energy on occupation number by approximate DFT approaches and discussed a simple, self-interaction-free, fix that restores the linearity. Mark Pederson presented a retrospective on computational challenges for wide-spread use of self-interaction corrections, discussing the physical significance of localized and canonical orbitals in applications of SIC to molecules and solids and the impact of full-scale implementation in application-oriented fields. Nicola Marzari discussed electronic structure challenges, some of which stem from the remnants of self-interaction, for trying to reach qualitative and quantitative

accuracy and ability to perform quantum simulations under realistic conditions. He suggested possible solutions for these challenges based on constrained DFT, extended Hubbard functionals, or on imposing a generalization of Koopmans' theorem. Klaus Capelle started from reviewing connections between DFT and model Hamiltonians, highlighting the many possible benefits that arise from using insights from DFT to study model Hamiltonians, and ideas arising from model Hamiltonians to improve functionals for DFT. He considered orbital-dependent functionals, the PZ-SIC, and compared results from six different levels of approximate implementation, ranging from simple post-LDA strategies to a full OEP, to available exact results. Stephan Kuemmel discussed the Kohn-Sham approach to the SIC using one global multiplicative potential and studied the effects of orbital localization and the physical reliability of the thus obtained eigenvalues of organic semiconductor molecules. Peter Kluepfel presented results of self-consistent calculations of PZ-SIC applied to GGA and LDA functionals for atoms, molecules and solids. The use was made of an efficient method to minimize the energy with respect to the orbitals, involving explicit unitary optimization. Olle Eriksson gave the last invited talk of Monday, briefly outlining the Lundin-Eriksson approach to SIC, then full-potential LMTO implementation of PZ-SIC and recent developments of DMFT.

The poster session was very lively and enjoyed by all the participants. A few minutes long oral introductions of the posters by their presenters were found very helpful in organizing one's viewing preferences. A special highlight of the evening was a cake presented to John Perdew and Alex Zunger (see the photos below), with the first page of their seminal SIC paper imprinted on the icing on the top of the cake. Since the CECAM Council had decided to fund the SIC meeting not as a regular workshop, but as a celebration event, we came to conclusion that a cake, would be a fitting tribute to the celebration. The cake was cut by Alex, with John's assistance, and as seen in the photograph below, both seem to have enjoyed the experience and, hopefully, the cake as well. The cake was large enough, so everybody could eat a piece of it, and the lucky ones could even get a taste of an equation or similar.

Axel Svane gave the first talk of the Tuesday morning presenting results of many applications to $4f$ and $5f$ electron solids, based on the PZ-SIC implementation within the LMTO-ASA band structure method, discussing localization/delocalization phenomena and valency. Thomas Schulthess presented early results from the PZ-SIC implementation in the full-potential LAPW code and discussed the importance of spherical vs. non-spherical issues in comparison with importance of the choice of the starting Wannier functions and energy minimization. Björn Baumeier started the sequence of talks related to the so-called pseudo-SIC approach for crystalline systems. Allesio Filippetti continued in the similar spirit, however concentrating on the applications to strongly correlated systems, outlining also the variational pseudo-SIC approach. Then Hisazumi Akai presented some results from the pseudo-SIC implementation in the KKR method, using the energy dependent functions, instead of projections on a fixed set of atomic functions. He also talked about EXX+RPA approach. Julie Staunton gave the last talk of the second day and described a combined approach of DLM with the so-called local SIC implementation in the KKR formalism. She presented results of its application to finite temperature magnetism in heavy rare earth and transition metal oxides (TMO), showing the existance of a well defined gap in the paramagnetic state of TMOs.

The late afternoon was spent on a few hours walk around the historic sights of the beautiful city of Chester. The day was finished with a "conference" dinner in The Ship Inn, overlooking the river Dee. It was a nice and pleasant event.

The first talk of the last day of the meeting was given by Adrienn Ruzsinszky on the non-empirical fully-nonlocal functionals for correlation, compatible with SI-free exact exchange. Her talk was followed by Eric Suraund's on time-dependent self-interaction free DFT. Takao Tsuneda talked about regional SIC of long-range corrected DFT. Aron Cohen discussed many electron self-interaction problem and the connection between self-interaction and strong correlation. Stefano Sanvito discussed the impact of self-interaction error on electronic transport across nanodevices based on an atomic/pseudo-SIC approach. The last talk of the meeting was by Nikitas Gidopoulos who discussed self-interaction free potentials from constrained density functional approximations.

The meeting was concluded with a two-hours long round table discussion well introduced and skillfully moderated by George Malcolm Stocks. The discussions were lively and useful, tackled many important issues of SIC implementations, importance of complex orbitals, minimization and transformation matrix optimizations, etc. There was also talk about establishing a SIC Club or a formal framework for validation and verification of SIC results obtained with different implementations. A follow-up meeting in a couple of years or so was also contemplated. All in all, it was a very interesting meeting, praised by many and assessed as very beneficial by all the participants.

Finally, the local administration of the meeting, the venue, food and all the services provided by the Ramada staff were very highly appreciated.

Programme

Sunday 18th September 2011

17:00 - 20:00 Arrival and Registration

Monday 19th September 2011

08:45 Walter Temmerman (Daresbury): CECAM Daresbury Node Director
and Vice-chair of Psi-k
Opening Remarks

Chair: Thomas Schulthess (Zurich)

09:00 John Perdew (Tulane)
"Rethinking the Perdew-Zunger Self-Interaction Correction,
after 30 Years"

09:45 Alex Zunger (Colorado)
"Predicting localization, delocalization and polaron behaviour
in insulators via restoration of the proper energy vs.
occupation (linear) dependence to DFT"

10:30 Coffee/Tea

11:00 M Pederson (Washington DC)
"Computational Challenges for Wide-Spread Use of Self-
Interaction-Corrections:A retrospective"

11:45 Nicola Marzari (Lausanne)
"Nothing works! Electronic-structure challenges in modelling
materials for energy applications" ("Three perspectives on
self-interaction - long-range charge transfer, short-range
hybridization, and photoemission levels")

12:30 Lunch

Chair: John Perdew (Tulane)

14:00 Klaus Capelle (Sao Paulo)
"Model Hamiltonians: A Theoretical Laboratory for DFT"

14:45 Stephan Kuemmel (Bayreuth)
"Kohn-Sham Self-interaction correction - a route to physically meaningful orbitals"

15:30 Coffee/Tea

16:00 Peter Klüpfel, Simon Klüpfel, Hildur Guðmundsdóttir and Hannes Jónsson (Reykjavik)

"Perdew-Zunger SIC and other orbital density dependent functionals"

16:45 Olle Eriksson (Uppsala)
"Recent attempts of self-interaction"

18:30 Food and Posters: Chair: Antonios Gonis (LLNL)

Tuesday 20th September 2011

Chair: Olle Eriksson (Uppsala)

09:00 A Svane (Aarhus)
"Self-interaction corrections of solids in the LMTO formalism"

09:45 Thomas Schulthess (Zurich)
"Non-spherical self-interaction corrections implemented within the all-electron LAPW method"

10:30 Coffee/Tea

11:00 Bjoern Baumeier (Mainz)
"Self-interaction corrected pseudopotentials for crystalline systems"

11:45 Alessio Filippetti (Cagliari)
"A variational approach to the study of strong-correlated oxides based on the self- interaction removal from local

density functional"

12:30 Lunch

Chair: Nicola Marzari (Lausanne)

14:00 Hisazumi Akai (Osaka)
"A pseudo-SIC implementation in the KKR code and applications"

14:45 Julie Staunton (Warwick)
"Magnetic and electronic structure at finite temperatures described ab-initio: disordered local moments and the self-interaction correction"

16:00 Walk around Chester + Dinner of the Event

Wednesday 21st September 2011

Chair: Mark Pederson (Washington DC)

09:00 Adrienn Ruzsinszky (Tulane)
"Nonempirical Fully-Nonlocal Density Functional for Correlation, Compatible with Self-Interaction Free Exact Exchange"

09:45 Eric Suraud (Toulouse)
"The Self Interaction Correction revisited"

10:30 Coffee/Tea

11:00 Takao Tsuneda (Yamanashi)
"Regional self-interaction corrections of long-range corrected DFT"

11:45 Aron Cohen (Cambridge)
"Connection between self interaction and strong correlation"

12:30 Lunch

Chair: George Malcolm Stocks (Oak Ridge)

14:00 Stefano Sanvito (Dublin)
"The self-interaction error in electronic transport across nanodevices"

14:45 Nikitas Gidopoulos (Didcot)
"Constraining density functional approximations to yield self-interaction free potentials"

15:30 Coffee/Tea + Round Table Discussion:
George Malcolm Stocks (ORNL) - Moderator

17:30 Closing Workshop

Participants

Prof Hisazumi Akai, Osaka University, Japan
Dr Bjoern Baumeier, Max Planck Institute for Polymer Research, Mainz, Germany
Dr Michael Brooks, STFC Daresbury Laboratory, UK
Prof Klaus Capelle, UFABC, Brazil
Prof Henry Chermett,e Univ. LYON 1, France
Dr Aron Cohen, University of Cambridge, UK
Dr Markus Daene, Oak Ridge National Laboratory, USA
Prof Olle Eriksson, Uppsala University, Sweden
Dr Arthur Ernst, MPI Halle, Germany
Dr Andrea Ferretti, CNR Istituto Nanoscienze, Modena, Italy
Dr Alessio Filippetti, CNR-IOM & University of Cagliari, Italy
Mr Guntram Fischer, Martin-Luther Universitt Halle, Germany
Mr Matthias Geilhufe, Martin-Luther Universitt Halle, Germany
Dr Nikitas Gidopoulos, ISIS, STFC Rutherford Appleton Laboratory, UK
Ms Hildur Guδmundsdóttir, Science Institute, University of Iceland
Prof Balazs Gyorffy, University of Bristol, UK
Mr Dirk Hofmann, University of Bayreuth, Germany
Ms Nina Kearsey, Imperial College London, UK
Dr Peter Klüpfel, Science Institute, University of Iceland
Mr Simon Klüpfel, Science Institute, University of Iceland
Prof Stephan Kuemmel, University of Bayreuth, Germany
Dr Martin Lueders, STFC Daresbury Laboratory, UK
Mr Keld Lundgaard, Technical University of Denmark
Prof Nicola Marzari, Theory and Simulations of Materials, EPFL,Switzerland
Dr Mark Pederson, Naval Research Laboratory, Washington DC, USA
Dr Chaitanya Das Pemmaraju, Trinity College Dublin, Ireland
Prof John P. Perdew, Tulane University, USA

Dr Leon Petit, STFC Daresbury Laboratory, UK
Ms Effat Rashed, University of Bristol, UK
Dr Adrienn Ruzsinszky, Tulane University, USA
Prof Stefano Sanvito, Trinity College Dublin, Ireland
Prof Thomas Schulthess, ETH Zurich, Switzerland
Prof Julie Staunton, University of Warwick, UK
Dr George Malcolm Stocks, Oak Ridge National Laboratory, USA
Prof Axel Svane, Aarhus University, Denmark
Prof Zdzislawa (Dzidka) Szotek, STFC Daresbury Laboratory, UK
Prof Walter Temmerman, STFC Daresbury Laboratory, UK
Dr Stanko Tomić, University of Salford, UK
Prof Takao Tsuneda, University of Yamanashi, Japan
Mr Jess Wellendorff, Technical University of Denmark
Prof Alex Zunger, Colorado University Boulder, USA