

CCP3 Working Group meeting, Rutherford Appleton Lab 24 Feb 2010

Attendees:

Phil Woodruff
Colin Norris
Sarnjeet Dhesi
Mike Finnis
Christine Bailey
Chris Nicklin
Keith Refson
Barbara Montanari
Leonardo Bernasconi
Andrew Fisher
Moritz Hoesch
Mark Read
Michele Warren
Barry Searle
Rob Lindsay
Stanko Tomic
Nic Harrison
Simon Crampin
Steven Kenny
John Purton

Apologies from:

Adrian Wander
Wendy Flavell
Rex Godby
G P Srivastava
Angelos Michealides
Werner Hofer
Roy Johnston

Talks

Leonardo Bernasconi gave a report on the development of TD-DFT within the CRYSTAL code: B3LYP+TD-DFT as implemented in CRYSTAL give very accurate electronic structures and photoemission and optical spectra. Static response properties will be released with CRYSTAL09. Full optical response spectra will be part of an intermediate release before the next main release.

Barry Searle presented an update on DLV: DLV3 has been released

Christine Bailey reported on the ROD project: Alpha version of ROD interfaced to DLV3 is available for both Linux and Windows (the latter not tested extensively). Users/potential users are request to provide feedback and suggestions for future extensions.

Comments on ROD from discussions:

- Current UK user base is 12 groups and this needs to expand. ROD will be made available to users on the beamline (which will come live later this year), and a tutorial is needed. The code is backward compatible.
- It would be useful for ROD to handle automatically cases where surface symmetry is different from bulk symmetry
- Are there opportunities for novel schemes for visualising/analysing the data, e.g. as multidimensional grids (e.g. as in neutron scattering community)
- Fitting and optimisation techniques could be improved (can we exploit developments in solving inverse problems within the mathematics community?)
- It would be useful to have an easy way to load structures into DLV (suggestions: from structure database, library of structures)

- Addition of 2D symmetry groups in DLV?
- Interactivity? Could it be made possible to move atoms, and see the effect?

Discussions

CCP3 personnel

- Adrian Wander has moved to a management position at Daresbury. Barbara Montanari has taken over as CCP3 Science Officer with Christine Bailey at Daresbury also taking over some CCP3 roles.

Developments at Diamond

The Working Group was updated on recent and forthcoming developments at DIAMOND.

- Nicklin: Possible need for grazing incidence small angle scattering code. Probably not suitable for DLV interfacing – different scale of system.
- Hoesch: ARPES beamline is scheduled to come online in ~3 years. The user community will be mainly those working on strongly correlated systems, and surface science. There is a potential need for codes that would be on the beamline available for users. Useful quantities from calculations are electronic band structures (bulk states, orbital symmetries), joint densities of states, and electron-phonon coupling. No strong demand for PHOTON to be updated.
- Dhesi: Principal beamline scientist for polarised soft X-rays. Would welcome support from theorists for calculations of magnetic properties, especially thin films and nanostructures. Several properties crucially dependent on spin-orbit coupling which would need to be included in the calculations.
- Demand for LEED codes expected to grow in the future. Possible development is to interface existing LEED codes (tensor LEED) with graphical interface. Current DL-LEED doesn't perform complete analysis.

Program Library

- Bailey will take over from Wander the job of responding to e-mail requests to CCP3
- It will be useful to gather statistics on user base for the codes, and make sure future usage properly recorded.
- Need to update the program library page on website. Indicate more clearly which codes CCP3 supports and add links to other codes that might be useful to the community.
- We should also use CCP3 program library page to make interested parties aware of other codes (e.g. those that require expert users) along with contacts. Inelastic tunneling code written as part of the last flagship proposal should be mentioned.
- Other codes that might be linked are Parker's code for surface calculations and Kenny's PLATO.

Composition of working group

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- New members are: Angelos Michaelides (UCL), Moritz Hoesch (Diamond), Steve Kenny (Loughborough), Paul Steadman (Diamond), Tien-lin Lee (Diamond)
- Other suggestions were discussed and will be contacted.

HECToR grant proposal

- Proposal drafted by Wander will be completed and submitted as a priority. Project will span a period of 3 years
- There is some scope for additional projects within the project scope, so anyone interested in participating is encouraged to get in touch immediately.
- Montanari will replace Wander and revise that aspect of the work plan.
- Proposal include a request for financial support for running costs of CCP3

- All co-authors need to update their parts and send material for the IMPACT statement
- Proposal will include plans for one or two workshops in the area of theoretical interpretation of experiments on surfaces and interfaces – need to involve calculations that can use efficiently a large number of processors. .

Flagship proposal

- The Working Group is reminded that all members may propose flagship projects.
- Flagship proposals have historically funded one or two PDRAs for 3 years.
- To have a chance of success will need to be science-led, and ideally strongly linked to experiment
- During discussions a possible theme emerged, focussed on : First principles calculations related to experiments that involve accurate prediction of excited states and problems requiring description that includes spin-orbit coupling. Would be potential strong link in to experiments at Diamond.

Future directions for CCP3

- Continue to improve usability of codes for experimentalists
- Diamond users would greatly benefit from theoretical support
- Include finite temperature effects in calculations. Possible topic for workshop?
- Consider organising a “Bring along a problem” workshop for experimentalists to describe problems they have that would benefit from theoretical input?
- Is there a demand for being able to performing optimisation across multiple datasets, from different experiments?

Workshops

CCP3 will organise a symposium on Computer simulation of surfaces and nanostructures at CMMP 2010 (Warwick, December). Suggestions for organisers, invited speakers, and plenary speakers (the latter urgent) are encouraged.

Input for CCPs steering panel meeting

Crampin will attend next meeting and report on CCP3 activities.

The next CCP3 working group meeting will be held in approximately 6 months with the option a South and a North site connected via videoconference link.

Summary of actions

1. **Bailey** will take over from Wander the job of responding to e-mail requests to CCP3
2. **Bailey** will gather statistics on user base for the codes
3. **Bailey** to update the program library page on website. Indicate more clearly which codes CCP3 supports and add links to other codes that might be useful to the community.
4. **Fisher** to identify appropriate manner of describing inelastic tunneling code written as part of the last flagship proposal and its availability on website.
5. **Crampin** to contact Parker and Kenny regarding linking to their codes via program page.
6. **Montanari** to invite potential new members to join working group.
7. **Crampin, Purton, Hofer, Tear** to send updates for HECToR proposal to Montanari as soon as possible
8. **Crampin, Purton, Hofer, Tear, Srivastava** to send material for IMPACT statement to Montanari as soon as possible

9. **All** to forward suggestions for possible workshops to be included within HECToR grant
10. **Montanari** to draft her part, and to manage preparation and submission of HECToR grant proposal
11. **All** to propose ideas for flagship grant proposals and to comment further on theme proposed at the meeting.
12. **STFC members** to investigate what implementation of spin-orbit coupling entails
13. **All** to send to Crampin any suggestions for organisers, invited speakers and plenary speakers for CMMP 2010 CCP3 symposium on surfaces and interfaces. Suggestions for plenary speakers are urgent.
14. **Crampin** to attend next CCPs steering panel meeting and inform them on our activity
15. **Montanari** to write and circulate minutes of this meeting
16. **Montanari** to organise next CCP3 working group meeting