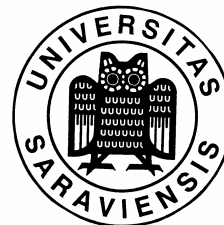


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Saarbrücken, 28.09.06

European Science Foundation

Re: Application for financial support for Scientific Meeting

Abstract

A 4-days conference on theoretical methods for the calculation of electronic and structural properties of materials shall be held in Saarbrücken, September 2007. It shall cover various aspects in the boarder region between chemistry and physics, thereby contributing to an increased transfer of knowledge between the two disciplines. The conference shall be held as a low-cost conference, making it, hopefully, also attractive to young scientists.

Conference title and schedule

In the middle of September 2007 I will organize a scientific conference on:

Large, Non-Biological Systems – Symposium for Theoretical Chemistry

Conference Programme

The conference shall take place at the University of Saarland, Saarbrücken, Germany, September 16th – September 20th 2007. The programme shall be:

	Sunday 16.09.	Monday 17.09.	Tuesday 18.09.	Wednesday 19.09.	Thursday 20.09.
Morning		Oral presentations	Oral presentations	Oral presentations	Oral presentations
Afternoon	Arrival + Registration	Oral presentations	Oral presentations	Excursion	Departure
Evening	Inofficial gathering	Posters + Buffet	Posters + Buffet	Conference dinner	

As seen, there will be 6 morning or afternoon sessions that each shall be split into 2 sessions. This gives 12 sessions that shall be devoted to various theoretical issues on the boarder between chemistry and physics:

1. Clusters (David Wales, Cambridge)
2. Polymers (Benoit Champagne, Namur)

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3. Surfaces (Joachim Sauer, Berlin)
4. Crystals (Karlheinz Schwarz, Wien)
5. Density functional theory (John Perdew, New Orleans)
6. Relativistic effects (Richard L. Martin, Los Alamos)
7. Local-increment methods (Hermann Stoll)
8. Coupled-cluster methods (Paul Jørgensen, Århus)
9. Excitations (?)
10. Dynamics (Dominik Marx, Bochum)
11. Solvation (Jacopo Tomasi, Italy)
12. Spin effects (Martin Kaupp, Würzburg)

The list contains also suggestions for people that shall be invited to give a keynote lecture on the various topics. I emphasize that the list is not yet complete and that none of the persons have been asked yet.

Participants

I expect that most of the participants will come from Germany, Austria, Switzerland, and France, but also participants from the other European countries are expected. Moreover, most likely there will be an admixture of theoretical chemists and theoretical physicists, thereby providing an excellent basis for exchanging information and experience between the two disciplines.

Goal

Traditionally, theoretical chemistry has focused on the study of small(er) molecules, whereas theoretical physics has concentrated on extended systems. During the last 20 years there has, however, been an increased change in both disciplines, whereby larger systems also have been of relevance and of interest to the chemistry community as have smaller systems to the physics community. This has led to an increased interaction between the two scientific disciplines, although less than ideally could be the case. The conference shall make a contribution to improve this interaction.

The conference shall focus on systems and methods that are of interest to both communities. In particular, methods with which electronic and structural properties can be determined shall be at the centre of the conference. In detail:

1. Clusters. These materials are typically larger than small molecules but not so large that they can be considered infinite, periodic crystals. From a theoretical point of view, one of the most difficult issues is that of determining the structure of the global total-energy minimum. This question shall be addressed by David Wales.
2. Polymers. Electronic and optical properties of conjugated polymers have been studied in chemistry, physics, and materials science for more than a quarter of a century. Among the most active in the field is Benoit Champagne.
3. Surfaces. Surfaces is one area where chemistry and physics meet, for instance in the study of catalytic processes. This shall be discussed by Joachim Sauer.
4. Crystals. This is traditionally the research field of physics and shall, therefore, here be included, too. Karlheinz Schwarz is the author of one of the most important computer codes in this field, WIEN2k.
5. Density functional theory. Whereas methods based on this theory for the longest time were applied in physics, it took some 20 years before they became established in chemistry. There are still a number of open issues about how various properties can be calculated with "chemical accuracy". John Perdew shall present a physicist's point of view on the chemistry problems.
6. Relativistic effects. For heavy elements, relativistic effects can not be ignored and have, in addition, surprising consequences. Their theoretical treatment is, however, not easy. Richard Martin has been working on these for many years and shall discuss his approaches and results.

7. Local-increment methods. This is a method from the chemistry community that finds increasing application in extended systems like crystals. Hermann Stoll plays a central role in their development.
8. Coupled-cluster methods. Such methods have first of all been developed and applied in the chemistry community but may also be of relevance for physics problems, in particular when correlation effects are important. Poul Jørgensen has for many years been involved in development and application of such methods.
9. Excitations. The study of excitations is significantly more complicated than that of ground-state properties. Therefore, also this issue shall be discussed at the conference.
10. Dynamics. Adding a time coordinate to the calculations increases the complexity of the calculations. Dominik Marx is one of those who have made the most significant contributions to this field, in particular concerning charge transport in hydrogen-bonded systems.
11. Solvation. Not always experiments are performed in the gas phase, whereas most calculations assume that the systems of interest exist in this phase. However, solvation effects may be important. Since many years, Jacopo Tomasi has developed and applied more different methods for studying for instance chemical reactions between molecules in a liquid phase.
12. Spin effects. Spin experiments (NMR and ESR, e.g.) are important for providing experimental information on structural and dynamical properties of systems. Their theoretical treatment requires very accurate calculations, which have been the field of research of Martin Kaupp for several years.

Besides these 12 overview lectures, a set of talks shall be provided in the form of contributed papers. I expect of the order of 3 shorter talks per session, i.e., in total 36 shorter talks.

Conference budget

I plan to organize the conference as a low-cost conference. This will make the conference attractive to young scientists, i.e., PhD students and post-docs. A rough estimate is that, except for hotel costs, the conference fee will be lower than 90 €. This does, however, not include the costs for invited speakers.

Therefore, I am applying for financial support for those.

Without knowing exactly what these persons would need, I estimate the average costs to be 1000 € / person, giving 12000 € costs for invited speakers. I expect to be able to cover about 50 % from other sources, and apply, therefore, for

6 000 €

to cover parts of the costs related to inviting the key-note speakers.

Curriculum vitae of the applicant

I am a Danish citizen, born 18.01.56 in Ajstrup Denmark.

1980: Diploma engineer from the Technical University of Denmark, Lyngby, Denmark

1982: PhD from the Technical University of Denmark, Lyngby, Denmark

1982 – 1986: Scientist at Max-Planck-Institute of Solid State Research, Stuttgart, Germany

1986 – 1989: Scientist at Nordita, Copenhagen, Denmark

1989 – 2000: Ass. Professor at Physical Chemical Institute, University of Konstanz, Germany

1994: Habilitation at the University of Konstanz in the Departments of Chemistry and of Physics

Since 2000: Professor of Theoretical and Physical Chemistry, University of Saarland, Saarbrücken, Germany

Recent publications of the applicant

In total about 160 scientific papers and 2 textbooks.

Among the papers:

Y. Dong, M. Burkart, M. Veith, and M. Springborg: *Electronic and structural properties of nanostructured HAIO*, J. Phys. Chem. B, 109 (2005) 22820-22829.

A. M. Asaduzzaman and M. Springborg: *Structural and electronic properties of Au, Pt and their bimetallic nanowire*, Phys. Rev. B 72 (2005) 165422 (8 pages).

P. Sarkar, M. Springborg, and G. Seifert: *A theoretical study of the structural and electronic properties of CdSe/CdS and CdS/CdSe core-shell nanoparticles*, Chem. Phys. Lett. 405 (2005) 103-107.

V. G. Grigoryan and M. Springborg: *Structural and energetic properties of nickel clusters: $2 \leq N \leq 150$* , Phys. Rev. B 70 (2004) 205415 (15 pages).

M. Springborg and R. C. Albers: *Charge and dimensionality effects on the properties of CaNiN*, Phys. Rev. B 69 (2004) 235115 (10 pages).

J. Tao, M. Springborg, and J. P. Perdew: *Properties of the exchange hole under an appropriate coordinate transformation*, J. Chem. Phys. 119 (2003) 6457-6464.

Yours sincerely,

(Prof. Dr. Michael Springborg)