

# **Proposal for an international workshop**

## **1. Title and purpose of the workshop**

Title: Ab initio Description of Iron and Steel (ADIS2006) Status and future challenges

The aim of the workshop is to bring together distinguished experts in ab-initio calculations and thermodynamic/kinetic modeling of metals. In particular, the meeting will deal on recent developments in accurately and efficiently modeling finite-temperature properties/processes and phase transitions.

Date: February 19-24, 2006

Web page: [adis-2006.mpie.de](http://adis-2006.mpie.de)

Announcement: Psi-k Newsletter July 29, 2005

Organizers:

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## **2. The scientific content, choice of time**

During the workshop various ab-initio approaches and thermodynamic/kinetic methods to model finite-temperature properties/processes and phase transitions will be discussed. Key experts in both fields have been invited to give tutorial-like lectures on recent methodological advances and future applicational challenges.

The aim of the meeting is the discussion and exchange of concepts for a combination of these approaches in order to describe realistic materials. A particular (but not exclusive) focus will be on iron, steel and metal alloys. The development of ab-initio based thermodynamic tools will be crucial to meet the increasing demand in fabricating novel alloys with tailormade properties such as e.g. light-weight high-strength steels in the car industry.

The workshop is organized by the Computational Materials Design department which has been recently established at the Max-Planck-Institute fuer Eisenforschung in Duesseldorf (Germany).

### **3. List of (confirmed) invited speakers**

D. Alfe (University College London, Great Britain)  
M. Asta (Northwestern University, USA)  
P. Bloechl (Clausthal Technical University, Germany):  
S. Bluegel (Research Center Jülich, Germany)  
G. Ceder (Massachusetts Institute of Technology, USA):  
P. Entel (University Duisburg-Essen, Germany):  
H. Eschrig (University Dresden, Germany):  
M. Faehnle (Max-Planck Institute Stuttgart, Germany):  
S. Mueller (University Erlangen-Nuernberg, Germany):  
M. Probert (University York, Great Britain)  
K. Schwarz (Technical University Vienna, Austria)  
F. Willaime (Sacley, France):

### **4. The participants**

The workshop is restricted to 40 participants.

About 15 experts in the fields of ab initio calculation and thermodynamic modeling have been/ will be asked to give 90-minute tutorial like presentations (incl. 15 minutes for discussion). All participants have the opportunity to present their results in poster sessions. A selected number of 30-minute oral contributions is planned.

A major part of the participants will be young scientists (PhD students and Postdocs).

### **5. Tutorial element**

A particular intention of the workshop is the transfer of knowledge from experts experienced with certain ab-initio approaches and thermodynamic/kinetic concepts to young scientists which are less familiar with these methods. To strengthen this element invited speakers have been asked to give their talks in a tutorial style. The program will provide ample time for each participant to present and discuss his or her own research.

### **6. Budget**

The expenses for the workshop are approximately 27,000 EUR. This includes the costs for conference center, accommodation and meals (~17,000 EUR), financial support for traveling (~7,000 EUR) and further costs (~3,000 EUR).

We would like to apply for 5,000 EUR from the ESF Psi-k Programme.

Together with the expected revenue from conference fees (~8,000 EUR), the confirmed money of co-sponsors (~4,000 EUR) and a financial contribution of the Max-Planck Society of max. 10,000 EUR, we will then be able to cover the costs.

### **7. Additional funding**

The Schloessmann foundation agreed to sponsor the conference fees for participants coming from the Max-Planck Society: ~ 4,000 EUR.

The Max-Planck institute for iron research Duesseldorf is willing to pay 10,000 EUR (incl. the conference fee for members of their institute).

We have applied for financial support from the Research Programme of the Research Fund for Coal and Steel of the European Commission.

### **8. Location**

The workshop takes place at Ringberg Castle (Bavaria, Germany). Since it is operated directly by the Max-Planck Society, the cost/performance ratio of this place is particularly favourable for us.

### **9. Participants from America**

Fortunately, two leading scientists from America have agreed to give a tutorial talk at our workshop. These are

- M. Asta (Northwestern University, USA)
- G. Ceder (Massachusetts Institute of Technology, USA)

To cover their travel expenses is a particular challenge for us. Any additional financial assistance would be appreciated.