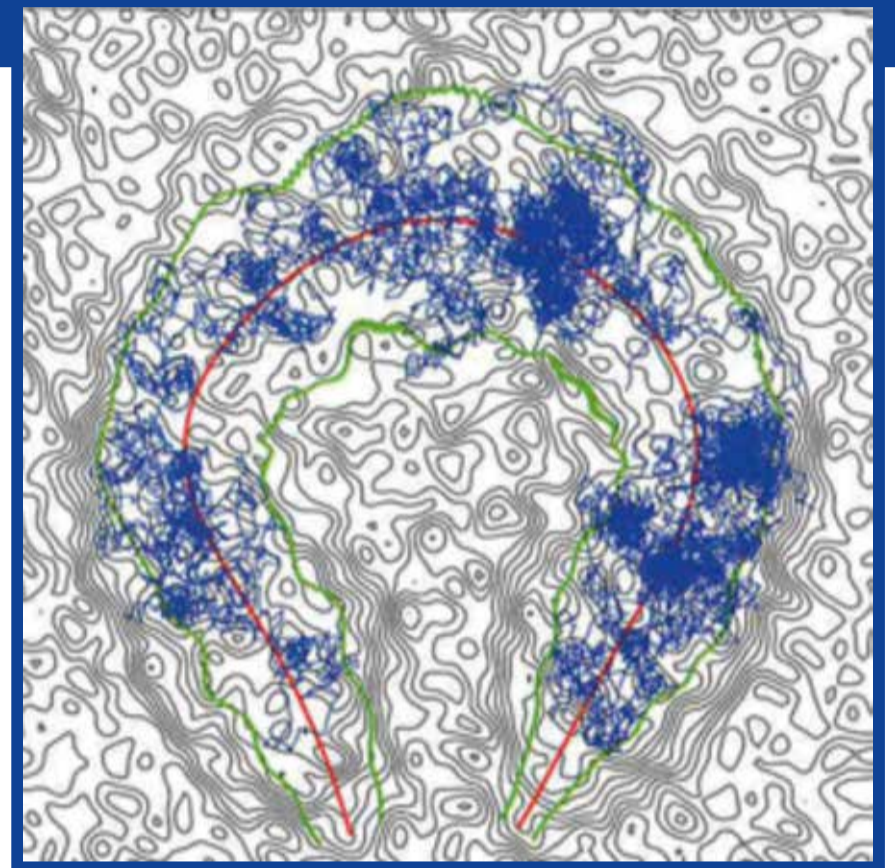




# Bridging-Time Scale Techniques and their Applications in Atomistic Computational Science

## Focus Workshop 12 - 15 September 2016

Since molecular dynamics can only access small time scales, new atomistic simulation techniques are required for kinetic processes such as diffusion, protein folding or crystal growth. A major challenge is to develop methods to explore free energy surfaces and transitions between states. The focus workshop will address such issues through a multidisciplinary approach involving scientists from different disciplines.



### Topics include

- Kinetic Monte Carlo simulations with and without pre-defined event lists and Wang-Landau methods
- Accelerated dynamics methods, eg hyperdynamics, temperature accelerated dynamics
- New developments in transition state theory
- Basin and other methods for low energy barrier problems
- Parallel algorithms including parallel replica dynamics
- Barrier height determination and reaction pathways
- Time acceleration through modification to potential energy surfaces
- Applications of the techniques in biology, chemistry, physics and engineering

### Invited speakers

Jacques Amar\* (US)  
Charlotte Becquart (FR)  
Josep Bofill\* (ES)  
Vasily Bulatov\* (US)  
Abhijit Chatterjee (IN)  
Weinan E (US)  
Kristen Fichthorn (US)  
Fei Gao\* (US)  
Graeme Henkelman (US)  
Charles Jaffe (US)  
Hannes Jonsson (IS)  
David Landau (US)  
Ju Li\* (US)  
Zshipan Lui (CN)  
Enrique Martinez (US)  
Ashlie Martini\* (US)  
Normand Mousseau (CA)  
Marcus Müller (DE)  
Maylise Nastar (FR)  
Shigenobu Ogata\* (JP)  
Per Olsson (SE)

Danny Perez (US)  
Wolfgang Quapp (DE)  
Roman Schubert (UK)  
Pratyush Tiwari (US)  
Gareth Tribello\* (UK)  
Art Voter (US)  
Holger Waalkens (NL)  
Haixuan Xu (US)  
*\* to be confirmed*

### Scientific coordinators

Matthias Posselt  
Dresden, Germany  
Roger Smith  
Loughborough, UK  
Blas Uberuaga  
Los Alamos, US

### Organisation

Amy Wright  
MPIPKS, Dresden

Applications received before 20 May will be considered preferentially.

Applications are welcome and should be made by using the application form on the event's web page. The number of attendees is limited. The registration fee for the focus workshop is 120 Euro and should be paid by all participants. Costs for accommodation and meals will be covered by the Max Planck Institute. Limited funding is available to partially cover travel expenses. Please note that childcare is available upon request.

### For further information please contact:

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