

CCP6 Workshop Molecular Potential Energy Surfaces in Many Dimensions

Aberdeen, Monday 30th June – Thursday 3rd July, 2008

PROGRAM

Monday

17:00 - 22:00 Registration

19:00 - 19:30 Bar open at 19:00 Dinner at 19:30

Tuesday

7:30 - 8:40 Breakfast

All talks in Meston Lecture Theatre 1

9:00 - 9:05 Mark Law Introduction

9:05 - 9:50 Peter Knowles Reduced electronic structure models
for large-molecule reactions

9:50 - 10:35 Tanja van Mourik Determining potential energy surfaces
for flexible peptides. Problems caused by
intramolecular BSSE and dispersion

10:35 - 11:00 Coffee

11:00 - 11:45 Horst Köppel Multi-mode quantum dynamics studies for multiple
intersections of potential energy surfaces.

11:45 - 12:30 Graham Worth Efficient Searching of Relevant Configuration Space:
Direct Dynamics and the DD-vMCG Method

12:45 Lunch

14:00 - 17:45 Excursion Crathes Castle, Gardens & Estate

18:00 - 18.20 Massimiliano Bartolomei Potential energy surfaces for $O_2(^3\Sigma_g^-) + O_2(^3\Sigma_g^-)$

18:20 - 18:40	Roberto Marquardt	Global analytical representations of PES in ammonia and CO/Cu(100)
19:00 - 20:00	Poster session + finger buffet	Venue: 'Chemistry Conference Room'
<u>Wednesday</u>		
7:30 - 8:40	Breakfast	
9:00 - 9:45	Kirk Peterson	The use of explicitly correlated methods for accurate potential energy surfaces
9:45 - 10:30	Claude Leforestier	The quest for a quantum water potential
10:30 - 11:00	Coffee	
11:00 - 11:45	Bastiaan Braams	High accuracy potential energy and dipole moment surfaces for water clusters
11:45 - 12:30	John Herbert	The role of the neutral water potential in determining the properties of anionic water clusters
12:45	Lunch	
14:00 - 14:45	Tucker Carrington	Some new neural network based tools for fitting potential surfaces
14:45 - 15:05	Richard Dawes	Interpolating moving least-squares methods for fitting potential energy surfaces: A strategy for efficient automatic data point placement in high dimensions
19:30	Conference Dinner	Foyer Restaurant, 82a Crown Street
<u>Thursday</u>		
7:30 - 8:40	Breakfast	
9:00 - 9:45	Attila Császár	Ab initio PESs and their utilization in variational computations.
9:45 - 10:30	Richard Wheatley	Recent progress in calculating atomistic potentials
10:30 - 11:00	Coffee	
11:00 - 11:45	Michael Collins	Potential energy surfaces and matrices for chemical reaction dynamics
11:45 - 12:30	Final Discussion	
12:45	Lunch	