Programme

QRS 2017	Monday July 3rd		Tuesday July 4th		Wednesday July 5th		Thursday July 6th
8:30 - 16:00	Registration	9:00 - 10:00	J. Bowman: Keynote Talk	9:00 - 10:00	ICCSA Keynote Talk		
9:00 - 9:30	ICCSA 2017 Official Opening	10:00 - 10:20	Coffee break	10:00 - 10:20	Coffee break		
9:30 - 10:30	ICCSA Keynote Talk		QRS4. Chair T. Stoecklin		QRS7. Chair F. J. Aoiz		
10:30 - 10:50	Coffee break	10:20 - 10:50	13. G. Lendvay	10:20 - 10:50	27. O. Roncero		Excursion (8:00 am)
	QRS1. Chair V. Aquilanti	10:50 - 11:20	14. L. Bonnet	10:50 - 11:20	28. T. Stoecklin		
		11:20 - 11:50	15. C. Coletti	11:20 - 11:50	29. B. Naduvalath		
10:50 - 10:55	QRS opening	11:50 - 12:20	16. R. Jaquet	11:50 - 12:20	30. T. González-Lezana		
10:55 - 11:25	1. A. Varandas						
11:25 - 11:55	2. G. Czakó						
11:55 - 12:25	3. T. J. Frankcombe						
12:30 - 13:30	Lunch	12:20 - 13:20	Lunch	12:20 - 13:30	Lunch		
	QRS2. Chair A. Laganà		QRS5. Chair L. Bonnet		QRS8. Chair N. Faginas Lago		
13:30 - 14:00	4. F. J. Aoiz	13:30 - 14:00	17. D. Babikov	13:30 - 14:00	31. E. Martínez-Núñez		
14:00 - 14:30	5. J. N. L. Connor	14:00 - 14:30	18. S. C. Althorpe	14:00 - 14:30	32. L. K. McKemmish		Excursion
14:30 - 15:00	6. D. Sokolovski	14:30 - 15:00	19. M. T. Cvitaš	14:30 - 15:00	33. M. Lara		
15.00 - 15:30	7. D. De Fazio						
15:30 - 15:50	Coffee break	15:00 - 15:20	Coffee break	15:00 - 15:20	Coffee break		
		15:20 - 15:50	20. R. Spezia				
		15:50 - 16:20	21. M. Ceotto				
	QRS3. Chair A. Varandas				QRS9. Chair F. Palazzetti		
15:50 - 16:20	8. C. Petrongolo		QRS6. Chair A. Lombardi	15:20 - 15:50	34. R. Welsch		
16:20 - 16:50	9. A. García-Vela			15:50 - 16:20	35. J. Kłos		
16:50 - 17:20	10. P. Honvault	16:20 - 16:50	22. T. Takayanagy	16:20 - 16:50	36. S. A. Vázquez		Excursion
17:20 - 17:50	11. M. Hochlaf	16:50 - 17:20	23. F. Huarte-Larrañaga	16:50 - 17:20	37. D. Skouteris		
17:50 - 18:20	12. T. Nagy	17:20 - 17:50	24. V. H. Carvalho-Silva	17:20 - 17:50	38. M. Mondelo Martell		
		17:50 - 18:20	25. P. García Jambrina				
18:20 - 19:00	Poster session	18:20 - 18:50	26. X. Shan				
19:00 - 22:00	ICCSA 2017 Welcome reception	19:00 - 23:00		19:00 - 23:00	Gala Dinner		

1. From a cost-effective wave function-based approach in electronic structure to accurate quantum dynamics
2. Dynamics and novel mechanisms of SN_2 reactions on ab initio analytical potential energy surfaces
3. Efficient ways to build potential energy operators
4. Elucidating the reaction mechanism through the Λ doublet ratio
5. How to derive a physically meaningful analytic S matrix from numerical S matrix data
6. Regge poles as a practical tool: towards software for analyzing resonance effects in reactive angular distribution
7. Benchmarking chemical reactivity in the deep tunneling regime: the ultra-cold behavior of the $F+H_2$ reactive system and its isotopic variants
8. Nonadiabatic effects in quantum reactive collisions
9. Quantum coherent control of the properties of a resonance state
10. Isotope and symmetry effects in collisions involving ozone as intermediate
11. Generation of accurate multi-dimensional potential energy surfaces of polyatomic molecular clusters and applications
12. Semiclassical quantization of rovibrational states of methane by adiabatic switching

Keynote Talk (Tuesday, July 4t^h, 09:000 am): Computational approaches to molecular Science

13. Dynamics of complex-forming bimolecular reactions
14. Semiclassical treatment of polyatomic reaction dynamics
15. Long range potential effects on the reactive and inelastic scattering in $OH+H_2$ collisions: a quantum-classical study
16. Investigations of non-adiabatic effects for a triatomic molecule: the use of a single potential energy surface with distance-dependent reduced masses for H_3^+
17. Mixed quantum/classical theory for rotationally and vibrationally inelastic scattering
18. Tunnelling in water clusters from instanton and path-integral simulations
19. Calculation of tunneling splittings in polyatomic molecules and clusters using instanton theory
20. Non-Statistical behaviors in gas phase uni- and bimolecular reactions. The role of chemical dynamics simulations
21. Quantum and semiclassical methods for molecular rate constants and vibrational spectra calculations
22. Frequency-domain and time-domain transition state spectroscopy of cyclooctatetraene
23. Quantum dynamics of H_2 in a carbon nanotube: timescale separation and resonance enhanced tunneling
24. Deformed transition-state theory: deviation from Arrehenius behavior and application to chemical reactions within the moderate tunneling regime
25. Interferences between reaction mechanisms unravelled using a quantum analogue to the classical deflection function
26. Full- and reduced-dimensionality semiclassical transition state theory: application to various chemical reactions
27. Reactive collisions at the cold temperatures of interstellar clouds: H_2CO+OH example
28. Vibrational sympathetic cooling of BaCl+ by Ca atoms: theoretical study
29. State-to-State chemistry and quantum dynamics of the ultracold K+ KRb reaction
30. Dynamics of reactive collisions in the interstellar medium
31. Methanol dimer formation drastically enhances hydrogen abstraction from methanol by OH at low temperature
32. Rmatreact: developing novel theoretical methodology to investigate ultra-cold atom-molecule collisions over deep potential wells
33. Dynamics of the $S(^1D)+o\text{-}D_2 \rightarrow SD+D$ reaction at low collision energies: revisiting the SH_2 system
34. Ultra-fast electronic decoherence caused by nuclear motion and a possible path to attochemistry
35. Photodissociation reaction of SO_2 and bound states on new ab initio potentials
36. Methyl cyanoformate decomposition: formation of HCN and HNC via concerted three-body dissociations
37. A diabatic electronic state system to describe the internal conversion of azulene
38. The role of tunneling on the diffusion rate of H_2 and D_2 along a narrow SWCN