

**ABSTRACTS OF THE PRESENTATIONS OF THE
XVIth QUANTUM REACTIVE SCATTERING WORKSHOP
4-9. September 2022.
Balatonföldvár, Hungary**

INTRODUCTION

The conference series on Quantum Reactive Scattering, popularly referred to as QRS, has over 30 years of history. It was initiated by David Clary and the first meeting was held in 1990. The number of participants is generally well below a hundred people, which allows intense exchange of ideas in a workshop atmosphere. The meeting has been organized in many countries, spreading from Japan to California:

1990 Cambridge, UK, David Clary (chair)

1994 Cambridge, Massachusetts, USA, Yan Sun and Michael Baer (chairs)

1995 Nottingham, UK, David Clary and David Manolopoulos (chairs)

1997 Telluride, Colorado, USA, Joel Bowman (chair)

1999 Perugia, Italy, Vincenzo Aquilanti and Antonio Laganà (chairs)

2001 Pasadena, California, USA, Aron Kuppermann (chair)

2003 San Lorenzo de El Escorial, Spain, Javier Aoiz and Luis Bañares (chairs)

2005 Santa Cruz, California, USA, Millard Alexander and Anne McCoy (chairs)

2007 Cambridge, UK, Stuart Althorpe (chair)

2009 Dalian, China, Dong-Hui Zhang and Ke-Li Han (chairs)

2011 Santa Fe, New Mexico, USA, Hua Guo (chair)

2013 Bordeaux, France, Laurent Bonnet and Pascal Larregaray (chairs)

2015 Salamanca, Spain, Octavio Roncero, Tomás González-Lezana, Susana Gómez-Carrasco, Lola González-Sánchez

2017 Trieste, Italy, Niyazi Bulut, Noelia Faginas Lago, Andrea Lombardi, Federico Palazzetti

2019 Saitama, Japan, Toshiyuki Takayanagi (chair)

The series was started at the time of intense development of quantum scattering methods applied to chemical reactions. Many of the new methods were presented and discussed at QRS meetings. In addition to exact quantum mechanical methods, semiclassical and quasiclassical methods were always present. During the years, the interest spread from “simple” reactions in triatomic systems to the dynamics of nonadiabatic processes and reactions in polyatomic systems, as well as to efficient algorithms to fit and interpolate potential energy surfaces.

Continuing this trend, at the XVIth workshop diverse fields are represented. The investigated systems are much more complex than in the early years. Some of the papers will discuss as accurate quantum mechanical methods as targeted previously, but numerous results obtained by quasiclassical trajectory calculations and new methods yielding rate coefficients directly will also be presented.

The current edition is organized with a one-year delay. Many of us will meet colleagues face-to-face after a two or three-year long hiatus. At this location a NATO Advanced

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Research Workshop on reaction dynamics was held in 2003, and many of the participants of that meeting convene now again here.

Thanks to Professor Antonio Laganà, editor of Virt&l-Comm, this collection of abstracts, organized in alphabetic order according to the presenting author's last name, appears before the meeting. Writing this introduction in advance, I hope that the participants will find this meeting as useful and enjoyable as the past editions of QRS were.

György Lendvay