# **Coherence and Control** in Chemistry

University of Leeds, United Kingdom 25–27 July 2011

# **FARADAY DISCUSSIONS** Volume 153, 2011

**RSC**Publishing

# Coherence and Control in Chemistry

Faraday Discussions

# www.rsc.org/faraday\_d

A General Discussion on Coherence and Control in Chemistry was held at the University of Leeds, Leeds, United Kingdom on 25th, 26th and 27th July 2011.

RSC Publishing is a not-for-profit publisher and a division of the Royal Society of Chemistry. Any surplus made is used to support charitable activities aimed at advancing the chemical sciences. Full details are available from www. rsc.org

# CONTENTS

ISSN 1359-6640; ISBN 978-1-84973-238-3

Coherence and Control in Chemistry

#### Cover

See Miller et al., Faraday Discuss., 2011, 153, 27-39.

This figure depicts the excitation of the dye molecule Rhodamine 110 with phase modulated femtosecond laser pulses, appearing nearly white, that leads to beautiful interferences in the induced coherences and enhanced population transfer—as depicted by the 2D spectra arising as peaks from the excited molecule.

Image reproduced by permission of Joerg M. Harms from *Faraday Discuss.*, 2011, **153**, 27.

# INTRODUCTORY LECTURE

9 Ultrafast laser control of electron dynamics in atoms, molecules and solids Matthias Wollenhaupt and Thomas Baumert

# PAPERS AND DISCUSSIONS

- Coherently-controlled two-dimensional spectroscopy: Evidence for phase induced long-lived memory effects
   Valentyn I. Prokhorenko, Alexei Halpin and R. J. Dwayne Miller
- 41 Electronic energy transfer in model photosynthetic systems: Markovian vs. non-Markovian dynamics Navinder Singh and Paul Brumer

- 51 Coherent control of single molecules at room temperature Daan Brinks, Richard Hildner, Fernando D. Stefani and Niek F. van Hulst
- 61 Exploring the role of phase modulation on photoluminescence yield D. G. Kuroda, C. P. Singh, Z. Peng and V. D. Kleiman
- 73 General discussion
- 93 Extracting dynamics of excitonic coherences in congested spectra of photosynthetic light harvesting antenna complexes Justin R. Caram and Gregory S. Engel
- 105 Multiconfigurational Ehrenfest approach to quantum coherent dynamics in large molecul systems Dmitrii V. Shalashilin
- 117 The influence of the optical pulse shape on excited state dynamics in provitamin D<sub>3</sub> Kuo-Chun Tang and Roseanne J. Sension
- 131 Wavepacket and potential reconstruction by four-wave mixing spectroscopy: preliminary application to polyatomic molecules David Avisar and David J. Tannor
- 149 Entanglement in interference-based quantum control: the wave function is not enough Moshe Shapiro and Paul Brumer
- 159 Searching for pathways involving dressed states in optimal control theory Philipp von den Hoff, Markus Kowalewski and Regina de Vivie-Riedle
- Photoelectron photoion coincidence imaging of ultrafast control in multichannel molecula dynamics
  C. Stefan Lehmann, N. Bhargava Ram, Daniel Irimia and Maurice H. M. Janssen
- 189 General discussion
- 213 A General control mechanism of energy flow in the excited state of polyenic biochromoph Tiago Buckup, Jürgen Hauer, Judith Voll, Regina Vivie-Riedle and Marcus Motzkus
- 227 Coherent control of vibrational transitions: Discriminating molecules in mixtures A. C. W. van Rhijn, A. Jafarpour, M. Jurna, H. L. Offerhaus and J. L. Herek
- 237 Coherent control of the motion of complex molecules and the coupling to internal state dynamics
  Paul Venn and Hendrik Ulbricht
- 247 Combining dissociative ionization pump-probe spectroscopy and *ab initio* calculations to interpret dynamics and control through conical intersections Spiridoula Matsika, Congyi Zhou, Marija Kotur and Thomas C. Weinacht
- 261 Nonadiabatic *ab initio* molecular dynamics including spin-orbit coupling and laser fields Philipp Marquetand, Martin Richter, Jesús González-Vázquez, Ignacio Sola and Leticia González
- 275 Dynamic stark control: model studies based on the photodissociation of IBr Cristina Sanz-Sanz, Gareth W. Richings and Graham A. Worth
- 293 General discussion

- 321 From molecular control to quantum technology with the dynamic Stark effect Philip J. Bustard, Guorong Wu, Rune Lausten, Dave Townsend, Ian A. Walmsley, Albert Stolow and Benjamin J. Sussman
- 343 Controlled redistribution of vibrational population by few-cycle strong-field laser pulses William A. Bryan, C. R. Calvert, R. B. King, J. B. Greenwood, W. R. Newell and I. D. Williams
- 361 Control of coherent excitation of neon in the extreme ultraviolet regime Jürgen Plenge, Andreas Wirsing, Christopher Raschpichler, Bernhard Wassermann and Eckart Rühl
- 375 Optical manipulation of coherent phonons in superconducting YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-8</sub> thin films Yasuaki Okano, Hiroyuki Katsuki, Yoshihiro Nakagawa, Hiroshi Takahashi, Kazutaka G. Nakamura and Kenji Ohmori
- 383 Femtosecond coherent control of thermal photoassociation of magnesium atoms Leonid Rybak, Zohar Amitay, Saieswari Amaran, Ronnie Kosloff, Michał Tomza, Robert Moszynski and Christiane P. Koch
- 395 General discussion

## CONCLUDING REMARKS

415 A perspective on controlling quantum phenomena Herschel Rabitz

## ADDITIONAL INFORMATION

- 419 Poster titles
- 421 List of participants
- 423 Index of contributors