University of Birmingham

Professor Graham Worth MA, DPhil, MRSC

Professor in Theoretical Chemistry

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About

Graham Worth is a Professor in Theoretical Chemistry. His main interest in the development of methods to solve the time-dependent Schrödinger equation for molecular systems. In particular he is a main developer of the powerful Multi-Configuration Time-Dependent Hartree (MCTDH) method, work he began as a Marie-Curie Research Fellow with Cederbaum in Heidelberg. The computer program is now used by many research groups and has provided benchmarks against which other methods are tested. He coordinates further developments of the program in collaboration with groups in Germany, France, Spain, Canada and Australia.

He chairs the Collaborative Computational Project on Molecular Quantum Dynamics (CCP6). In addition to methodological development, he is recognised internationally for his studies of ultrafast photochemistry and non-adiabatic effects and is regularly invited to present his work at national and international meetings.

Group Web Pages (http://www.stchem.bham.ac.uk/~worthgrp)

Qualifications

- DPhil in Chemistry, University of Oxford, 1992
- BA (Hons) in Chemistry, University of Oxford, 1989

Biography

After obtaining his BA in Oxford, Graham Worth studied for a doctorate there under the supervision of Prof. W. Graham Richards in the field of computation chemistry, calculating the thermodynamics of biochemical systems with applications to tautomerism in solution and phosphorylation in an enzyme. In Oct 1992 he then went on to a postdoctoral position at the European Molecular Biology Laboratory (EMBL), Heidelberg, in the group of Dr. Rebecca Wade to perform further studies on protein dynamics.

In Jan. 1994 he moved to the group of Prof. Lenz Cederbaum at the University of Heidelberg, first on an E.U. Human Capital and Mobility (later called Marie-Curie) Fellowship then on funding from the DFG and the VW Stiftung. Here he moved into the field of accurate quantum dynamics studies of small molecules and the development of the MCTDH program.

In Jan 2001 he joined the group of Prof. Mike Robb at King's College London as a Research Fellow to look at developing direct dynamics methods for the study of photochemistry. From Sept. 2003 he became a lecturer there and a Visiting Research Fellow at Imperial College, London. On the closure of the Chemistry Department at King's in May 2005, he moved to Birmingham as a University Research Fellow. He is now a Professor.

Teaching

Teaching Programmes

- BSc Chemistry
- MSci Chemistry

Postgraduate supervision

PhD Supervision in theoretical quantum dynamic

Research

RESEARCH THEMES

- Non-adiabatic effects in photochemistry
- Quantum dynamics using the MCTDH Algorithm
- Controlling chemistry using laser fields - coherent contro

Publications

Book

- H.-D. Meyer, F. Gatti, and G. A. Worth, editors. M C T D H: Basic Theory, Extensions, and Applications to Multidimensional Quantum Dynamics. VCH, Weinheim, Germany, 2009.

Selected Review Articles

- G. A. Worth and C. Sanz Sanz. Guiding the time-evolution of a molecule: Optical control by computer. PCCP, 12:15570, 2010.

- G. A. Worth, H.-D. Meyer, H. Koppel, L. S. Cederbaum, and I. Burghardt. Using the MCTDH wavepacket propagation method to describe multimode nonadiabatic dynamics. Int. Rev. Phys. Chem., 27:569, 2008.
- G. A. Worth, M. A. Robb, and B. Lasorne. Solving the time-dependent Schrodinger equation for nuclear motion in one step: Direct dynamics of nonadiabatic systems. Mol. Phys., 106:2077, 2008.
- G. A. Worth and L. S. Cederbaum. Beyond Born-Oppenheimer: Conical intersections and their impact on molecular dynamics. Ann. Rev. Phys. Chem., 55:127, 2004.
- G. A. Worth and M. A. Robb. Applying direct molecular dynamics to nonadiabatic systems. Adv. Chem. Phys., 124:355, 2002.

Selected Articles

- D. Mendive-Tapia, B. Lasorne, G. A. Worth, M. J. Bearpark, and M. A. Robb. Controlling the mechanism of fulvene S1/S0 decay: Switching o_ the stepwise population transfer. PCCP, 12:15725, 2010.
- M. Assmann, C. Sanz Sanz, G. P_erez-Hern_andez, G. A.Worth, and L. Gonzalez. Excited state dynamics of a model asymmetric molecular rotor: a fourdimensional study on 2-cyclopentylidene-tetrahydrofuran. Chem. Phys., 77:86, 2010.
- T. J. Penfold and G. A. Worth. The effect of molecular distortions on spin orbit coupling in simple hydrocarbons. Chem. Phys., 375:58, 2010.
- T. J. Penfold, G. A. Worth, and C. Meier. Local control of multidimensional dynamics. PCCP, 12:15616, 2010.
- C. S. M. Allan, B. Lasorne, G. A. Worth, and M. A. Robb. A straightforward method of analysis for direct quantum dynamics: Application to the photochemistry of a model cyanine. J. Phys. Chem. A, 114:8713, 2010.
- R. S. Minns, D. S. N. Parker, T. J. Penfold, G. A. Worth, and H. H. Fielding. Competing ultrafast intersystem crossing and internal conversion in the “channel 3" region of benzene. PCCP, 12:15607, 2010.
- D. Asturiol, B. Lasorne, G. A. Worth, M. A. Robb, and L. Blancafort. Exploring the sloped-to-peaked S2/S1 seam of intersection of thymine with electronic structure and direct quantum dynamics calculations. PCCP, 12:4949, 2010.
- Frankcombe T. J., M. A. Collins, and Worth G. A. Converged quantum dynamics with modied Shepard interpolation and Gaussian wave packets. Chem.Phys. Lett., 489:242, 2010.
- M. Araujo, B. Lasorne, A. L. Magalhes, G. A. Worth, M. J. Bearpark, and M. A. Robb. The molecular dissociation of formaldehyde at medium photoexcitation energies: a quantum chemistry and direct quantum dynamics study. J. Chem. Phys., 131:144301, 2009.
- T. J. Penfold and G. A. Worth. A model Hamiltonian to simulate the complex photochemistry of benzene II. J. Chem. Phys., 131:064303, 2009.
- D. S. N. Parker, R. S. Minns, T. J. Penfold, G. A. Worth, and H. H. Fielding. Ultrafast dynamics of the S1 excited state of benzene. Chem. Phys. Lett., 469:43, 2009.