

PUBLICATIONS

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BOOK

- [1] *12 × 12 Schlüsselkonzepte zur Mathematik*, with O. Deiser, E. Vogt, and D. Werner, Spektrum Akademischer Verlag, 2011.

PEER-REVIEWED JOURNALS IN MATHEMATICS

- [1] *Computing expectation values for molecular quantum dynamics*, with S. Röblitz, SIAM J. Sci. Comput. 32, 2010, pp. 1465–1483
- [2] *Semiclassical resonances for a two-level Schrödinger operator with a conical intersection*, with S. Fujie and L. Nédélec, Asymp. An. 65, 2009, pp. 17–58.
- [3] *Monte Carlo sampling of Wigner functions and surface hopping quantum dynamics*, with S. Kube and M. Weber, J. Comput. Phys. 228, 2009, pp. 1947–1962.
- [4] *Propagation through generic level crossings: a surface hopping semigroup*, with C. Fermanian-Kammerer, SIAM J. Math. An. 40(1), 2008, pp. 103–133.
- [5] *A rigorous surface hopping algorithm for conical crossings*, with T. Swart and S. Teufel, Commun. Math. Sc. 5(4), 2007, pp. 789–814.
- [6] *Propagation through conical crossings: an asymptotic semigroup*, with S. Teufel, Comm. Pure Appl. Math. 58(9), 2005, pp. 1188–1230.
- [7] *Wigner measures and codimension two crossings*, with C. Fermanian Kammerer, J. Math. Phys. 44(2), 2003, pp. 507–527.
- [8] *An overlapping domain decomposition preconditioner for a class of discontinuous Galerkin approximations of advection-diffusion problems*, with A. Toselli, Math. Comp. 72, 2003, pp. 1215–1238.

PEER-REVIEWED JOURNALS IN CHEMISTRY/PHYSICS

- [1] *Single switch surface hopping for molecular quantum dynamics* with C. Fermanian Kammerer, to appear in J. Math. Chem.

- [2] *Initial state dependence of coupled electronic and nuclear fluxes in molecules* with A. Kenfack, F. Marquardt, G. Paramonov, I. Barth, B. Paulus, Phys. Rev. A 81, 2010, 052502, (7 pp.)
- [3] *Trigonometric pulse envelopes for laser induced quantum dynamics*, with I. Barth, J. Phys. B: At. Mol. Opt. Phys. 42, 2009, 235101 (8 pp.)
- [4] *Single switch surface hopping for a model of pyrazine*, with T. Swart, J. Chem. Phys. 129, 2008, 034302 (8 pp.)
- [5] *Single switch surface hopping for molecular dynamics with transitions*, with C. Fermanian Kammerer, J. Chem. Phys. 128, 2008, 144102 (9 pp.)

PUBLICATIONS IN PROCEEDINGS

- [1] *Adiabatic approximation for quantum systems responding to laser pulses*, Classical and Quantum Mechanical Models of Many-Particle Systems (ed. A. Arnold, C. Cercignani, L. Desvillettes), Oberwolfach Report 54, 2006, p. 3249.
- [2] *Energy level crossings in molecular dynamics*, with F. Bornemann and T. Swart, Analysis, Modeling, and Simulation of Multiscale Problems (ed. A. Mielke), 2006, pp. 581–598.
- [3] *Laser control of nuclear and electron dynamics: bond selective photodissociation and electron circulation*, with I. Barth, L. González, J. Manz, and T. Rozgonyi, Coherent Control of Molecules CCP6, (ed. B. Lasorne and G. A. Worth), 2006, pp. 18–27.
- [4] *Convergence of some two-level overlapping domain decomposition preconditioners with smoothed aggregation coarse spaces*, with A. Toselli, Recent Developments in Domain Decomposition Methods, Lecture Notes in Computational Science and Engineering **23**, 2002, pp. 95–117.
- [5] *Overlapping preconditioners for discontinuous Galerkin approximations of second order problems*, with A. Toselli, Proceedings of the 13th International Conference of Domain Decomposition, 2001.

DISSERTATION

- [1] *Conical crossings in molecular dynamics*, PhD thesis at Technische Universität München, June 2004.

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