Publication list

Articles in peer-reviewed journals 1998-2004

1. Doppler effects in x-ray Raman scattering. F.Gel'mukhanov, H.Ågren, and P. Sałek. Phys.Rev. A **57**, No 4, 2511-2526 (1998)

2. Competition between decay and dissociation of core-excited carbonyl sulfide studied by x-ray scattering. M. Magnusson, J. Guo, C. Såthe, J.-E. Rubensson, J. Nordgren, P. Glans, L. Yang, P. Sałek and H. Ågren. Phys. Rev. A **59** No. 6, 4281-4287 (1999)

3. Duration of x-ray Raman scattering. Faris Gel'mukhanov and Paweł Sałek and Timofei Privalov and Hans Ågren. Phys. Rev. A **59** No. 1, 380-389 (1999)

4. Dynamics of Inner Shell Resonant Raman Scattering. H. Ågren, F. Gel'mukhanov, and P. Sałek. J.of the Jap. Society for Synchrotron Radiation Research,**12**, No 4,257-267 (1999)

5. Generalized Frank-Condon principle for resonant photoemission. Paweł Sałek and Faris Gel'mukhanov and Hans Ågren and Olle Björneholm and Svante Svensson. Phys. Rev A **60** No. 4 2786-2791 (1999)

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10. Resonant X-ray Raman scattering involving avoided crossings in the final state potential energy curves. P. Sałek, R.F. Fink, F. Gel'mukhanov, M.N. Piancastelli, R. Feifel, M. Bäßler, S. L. Sörensen, C. Miron, H. Wang, I. Hjelte, O. Björneholm, A. Ausmees, S. Svensson, and H. Ågren. Phys. Rev. A, **62**, 062506 (2000)

11. X-ray Raman scattering under pulsed excitation. F. Gel'mukhanov, P. Sałek, A. Shalagin, and H. Ågren. J. Chem. Phys. **112**, No 13, 5593-5603 (2000)

12. Dynamical suppression of atomic peaks in resonant dissociative photoemission. P. Sałek, V. Carravetta, F. Kh. Gel'mukhanov, H. Ågren, B. Schimmelpfennig, M. -N. Piancastelli, S. L. Sorensen, R. Feifel, I. Hjelte, M. Bässler, S. Svensson O. Björneholm, and A. Naves de Brito. Chem. Phys. Letters, 343, 332 (2001).

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*,** 15. Density-functional theory of linear and nonlinear time-dependent molecular properties. P. Sałek, O. Vahtras, T. Helgaker, and H. Ågren. J. Chem. Phys. 117, 9630 (2002).

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** 17. Calculations of two-photon absorption cross sections by means of density functional theory. P. Sałek, O. Vahtras, J.-D. Guo, Y. Luo, T. Helgaker, and H. Ågren.. Chem. Phys. Lett., 374 (2003) 446.

** 18. Density functional theory of nonlinear triplet response properties with applications to phosphorescence. I. Tunell, Z. Rinkevicius, O. Vahtras, P. Sałek, T. Helgaker, and H. Ågren. J. Chem. Phys. 119, 11024 (2003)

* 19. Dynamical properties of X-ray Raman Scattering. P. Sałek, A. Baev, F. Gel'mukhanov and H. Ågren. Phys. Chem. Chem. Phys., 5, 1-11 (2003)

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26. A comparison of DFT and coupled-cluster frequency-dependent polarizabilities and hyperpolarizabilities. P. Sałek, O. Vahtras, H. Ågren, T. Helgaker, D. Jonsson, and J. Gauss. Submitted.

*,** 27. Linear scaling formation of the Kohn-Sham Hamiltonian: application to the calculation of excitation energies and polarizabilities of large molecular systems. M. A. Watson, P. Sałek, P. Macak, T. Helgaker. Submitted to J. of Chem. Phys.

*,** 28. The calculation of indirect nuclear spin–spin coupling constants in large molecules. M. A. Watson, P. Sałek, P. Macak, M. Jaszuński, T Helgaker. Chemistry - A European Journal, 00, 000 (2004).

*,** 29. Calculations of static and dynamic polarizabilities of excited states by means of density functional theory. B. Jansik, D. Jonsson and P. Sałek. Submitted.

*,** 30. The trust-region self-consistent field method: Towards a black-box optimization in Hartree–Fock and Kohn–Sham theories. L. Thøgersen, J. Olsen, D. Yeager, P. Jørgensen, P. Sałek and T. Helgaker. J. of Chem. Phys. 00, 000 (2004).

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* 32. A wave-packet technique to simulate resonant X-ray scattering cross sections. Paweł Sałek. Comp. Phys. Comm. 150 (2003) 85-98

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Developed, publically available programs

1. RAM – a program for calculation of resonant X-ray scattering cross section. See also article no. 26.

2. Co-author of DALTON 2.0 (to be released Jun 2004). See `http://www.kjemi.uio.no/software/dalton/dalton.html`

Popular-science articles

1. Some Perspectives on Quantum Modelling of Molecular Materials. Paweł Sałek, Hans Ågren and Trygve Helgaker. KTH-Parallel Computer Center yearly report 2003.