

Publications, Posters, Invited Lectures.

Publications:

Wolfhard Koch and Friedrich Franz Seelig:
Extended HÜCKEL Calculations for the Interchain vs. Intrachain Coupling
of One-dimensional Conductors.
Molecular Crystals and Liquid Crystals **121** (1985), 371.

Wolfhard Koch:
*Extended-HÜCKEL-Berechnung der Energiebandstruktur
von Übergangsmetallverbindungen mit eindimensionaler Kristallgeometrie.*
Thesis, Universität Tübingen (1986).

Wolfhard Koch and Friedrich Franz Seelig:
Symmetry Orbitals for One-electron Band-structure Computations
of One-dimensional Crystals.
International Journal of Quantum Chemistry **32** (1987), 249-264.

Wolfhard Koch and Friedrich Franz Seelig:
Extended-HÜCKEL Energy Band Structures of Transition Metal Compounds
with One-Dimensional Crystal Geometries.
Basic Equations and Computational Results
for Bis(2,5-dimethyl-N,N'-dicyanoquinonediimine) copper(I).
Zeitschrift für Naturforschung **42a** (1987), 875-888.

Wolfhard Koch:
Extended-HÜCKEL Energy Band Structures of Organometallic Compounds
with One-Dimensional Crystal Geometries.
Computational Results
for Bis(2,5-dimethyl-N,N'-dicyanoquinonediimine) copper, -silver, and lithium.
Zeitschrift für Naturforschung **45a** (1990), 148-156.

Wolfhard Koch:
Neglect of Diatomic Differential Overlap (NDDO)
in Non-Empirical Quantum Chemical Orbital Theories.
Zeitschrift für Naturforschung **48a** (1993), 819-828.

Wolfhard Koch:
Simplified Non-Empirical Unrestricted HARTREE-FOCK Approximation (SUHF)
for the Calculation of Electronic Ground State Properties of Molecules
with Closed and Open Valence Shells.
I. Method.
Zeitschrift für Naturforschung **48a** (1993), 829-833.

Wolfhard Koch, Klaus Neymeyr, Markus Pernpointner, Barbara Schaper, and Klaus
Strecker:
Simplified Non-Empirical Unrestricted HARTREE-FOCK Approximation (SUHF)
for the Calculation of Electronic Ground State Properties of Molecules
with Closed and Open Valence Shells.
II. Diatomic Molecules.
Zeitschrift für Naturforschung **48a** (1993), 834-839.

Hartmut B. Stegmann, Thomas Jülich, Ulrike Höfler, Paul Schuler, Wolfhard Koch, Karsten Krohn and Astrid Eickhoff:

Synthesis, EPR, ENDOR and TRIPLE Resonance Investigations of Anthracycline-Related Semiquinones.

Magnetic Resonance in Chemistry **31** (1993), 468-471.

Wolfhard Koch:

On RÜDENBERG's Integral Approximations and Their Unrestricted and Combined Use in Molecular Orbital Theories of HARTREE-FOCK Type.

International Journal of Quantum Chemistry **76** (2000), 148-160.

(RUEDENBERG-Festschrift)

Posters:

Wolfhard Koch and Friedrich Franz Seelig:

Extended HÜCKEL Calculations for the Interchain vs. Intrachain Coupling of One-dimensional Conductors.

International Conference on the Physics and Chemistry of Low-Dimensional Synthetic Metals

and *International C.N.R. Symposium on Applications and Prospects of Synthetic Metals*,

Abano Terme (Italy), 17-22 June 1984.

Wolfhard Koch and Friedrich Franz Seelig:

Extended-HÜCKEL-Bandstrukturen eindimensionaler Komplexpolymere des Eisens und Kobalts.

Wolfhard Koch and Dietrich Hoffmann:

On RÜDENBERG's Integral Approximations.

34th Symposium for Theoretical Chemistry on Large Molecules,

Gwatt-Zentrum am Thunersee (Switzerland), 20-24 September 1998.

Invited Lectures:

- Universität Düsseldorf, Institut für Theoretische Chemie (at invitation of Prof. Schmidtke).
- Universität Stuttgart, Institut für Theoretische Chemie (at invitation of Prof. Preuß).
- Universität Tübingen, "Kann Chemie auf Physik reduziert werden?" *Studium generale*: "Chemie an der Schwelle des 21. Jahrhunderts", 24 November 1999 (at invitation of Prof. Häfelinger).
Video: <http://timms.zdv.uni-tuebingen.de>
- Universität Münster, Philosophisches Seminar, 15 February 2001 (at invitation of Prof. Hoyer).
- Universität Heidelberg, Institut für Theoretische Chemie, 27 May 2002 (at invitation of Prof. Cederbaum).
- Gustav-Siewerth-Akademie, Weilheim-Bierbronn: "Zur Problematik der Freiheit aus der Sicht der Quantenphysik", 20 September 2002 (at invitation of Prof. Hoyer, Universität Münster).
- Eidgenössische Technische Hochschule Zürich, Pharmazeutische Chemie (at invitation of Prof. Folkers).