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List of publications

M. Swart, M. van den Bosch, H.J.C. Berendsen, G.W. Canters and J.G. Snijders
“Active Site Geometries of Copper Proteins Obtained with a QM/MM Approach”
in preparation

F.C. Grozema, L. P. Candeias, M. Swart, P.Th. van Duijnen, J. Wildeman, G. Hadziioanou, L.D.A. Siebbeles and J.M. Warman
“Theoretical and Experimental Studies of the Opto-Electronic Properties of Positively Charged Oligo(Phenylene Vinylene)s: Effects of Chain Length and Alkoxy Substitution”
J.Chem.Phys. (2002) *submitted*

R.A. Steiner, M. Swart, J.G. Snijders and B.W. Dijkstra
“Density Functional Theory Investigation of the Reaction Mechanism of *A. japonicus* 2,3QD”
in preparation

M. Swart, M. van den Bosch, H.J.C. Berendsen, G.W. Canters and J.G. Snijders
“Calculations on the Spectral Characteristics of Copper Proteins”
in preparation

M. Swart
“AddRemove: a New Link Model for Use in QM/MM Studies”
Int.J.Quant.Chem. (2002) *accepted*

L. Jensen, M. Swart, P.Th. van Duijnen and J.G. Snijders
“Medium Perturbations on the Molecular Polarizability Calculated within a Localized Dipole Interaction Model”
J.Chem.Phys. (2002) *submitted*

M. Remko, P.Th. van Duijnen and M. Swart
“Theoretical Study of Molecular Structure, Tautomerism, and Geometrical Isomerism of N-Methyl and N-Phenyl Substituted Cyclic Imidazolines, Oxazolines and Thiazolines”
Phys.Chem.Chem.Phys. (2002) *in press*

P.Th. van Duijnen, A.H. de Vries, M. Swart and F.C. Grozema
“Polarizabilities in the Condensed Phase and the Local Fields Problem. A Direct Reaction Field Formulation”
J.Chem.Phys. (2002) *submitted*

M. Swart, M. van den Bosch, H.J.C. Berendsen, G.W. Canters and J.G. Snijders
“IntraFF: Obtaining Reliable Force Constants from Quantum Chemical Calculations”
to be submitted

M. Swart, M. van den Bosch, H.J.C. Berendsen, G.W. Canters, A.E. Mark and J.G. Snijders
“Modelling of the Redox Potential of Copper Proteins: Density Functional Theory and Molecular Dynamics Results for *Wildtype* and Mutated Azurin”
to be submitted

M. Swart, R.W.J. Zijlstra, F.C. Grozema, J.G. Snijders and R.M. Kellogg
“Asymmetric Addition of Dialkylzincs to Aldehydes Studied by High-Level Ab Initio Calculations. Similarities and Differences between Aminoalcohol and Aminothiols Promoted Reactions”
to be submitted

M. Swart and P.Th. van Duijnen
“DRF90: a Polarizable Force Field”
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- T. la Cour Jansen, M. Swart, L. Jensen, P.Th. van Duijnen, J.G. Snijders and K. Duppen
“Collision Effects in the Nonlinear Raman Response of Liquid Carbon Disulfide”
J.Chem.Phys. **116** (2002) 3277-3285
- R.W.J. Zijlstra, F.C. Grozema, M. Swart, B.L. Feringa and P.Th. van Duijnen
“Solvent Induced Charge Separation in the Excited States of Symmetrical Ethylene: a Direct Reaction Field Study”
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