

LCOAO publications

(2023)

1. J. Spanget-Larsen: "On Bridging the Gap Between Extended Hückel and NDO LCAO-MO Theories", *Theor. Chim. Acta* **55**, 165-172 (1980).
2. J. Spanget-Larsen: "Breakdown of the One-Electron Picture of Ionization for Hydrocarbon π Systems", *Croat. Chem. Acta* **56**, 991-1010 (1984).
3. J. Spanget-Larsen: "The Alternant Hydrocarbon Pairing Theorem and All-Valence Electrons Theory. An Approximate LCOAO Theory for the Electronic Absorption and MCD Spectra of Conjugated Organic Compounds. 1." *Croat. Chem. Acta* **104**, 711-717 (1986).
4. J. Waluk, A. Mordziński, J. Spanget-Larsen, E. W. Thulstrup: "The Electronic Spectrum of Benz[*a*]anthracene. Linear and Magnetic Circular Dichroism and Fluorescence Polarization Studies", *Chem. Phys.* **116**, 411-420 (1987).
5. J. Spanget-Larsen, J. Waluk, E. W. Thulstrup: "Electronic States of Chrysene. Linear and Magnetic Circular Dichroism and Quantum Chemical Calculations", *J. Phys. Chem.* **94**, 1800-1806 (1990); Erratum: **94**, 6926 (1990).
6. J. Spanget-Larsen, J. Waluk, S. Eriksson, E. W. Thulstrup: "Electronic States of Benzo[*a*]pyrene. Linear and Magnetic Circular Dichroism, Polarized Fluorescence, and Quantum Chemical Calculations", *J. Amer. Chem. Soc.* **114**, 1942-1949 (1992).
7. K. B. Andersen, J. Spanget-Larsen: "Electronic transitions and intramolecular hydrogen bonding in Anthralin. UV-VIS linear dichroism spectroscopy and quantum chemical calculations", *Spectrochim. Acta A* **53**, 2615-2625 (1997).
8. J. Spanget-Larsen: "The alternant hydrocarbon pairing theorem and all-valence electrons theory. An approximate LCOAO theory for the electronic absorption and MCD spectra of conjugated organic compounds. 2." *Theoret. Chem. Acc.* **98**, 137-153 (1997).
9. S. Møller, K. B. Andersen, J. Spanget-Larsen, J. Waluk: "Excited-state intramolecular proton transfer in anthralin. Quantum chemical calculations and fluorescence spectra", *Chem. Phys. Lett.* **291**, 51-56 (1998)
10. K. B. Andersen, "Electronic states of naphthazarin and related compounds. UV-VIS linear dichroism and quantum chemical model calculations", *Acta Chem. Scand.* **53**, 222-229 (1999)
11. J. Spanget-Larsen, D. Liang, E. Chen, E. W. Thulstrup: "Assignment of the IR and UV spectra of dibenzofuran: Linear dichroism spectroscopy and quantum chemical calculations", *Asian Chem. Lett.* **4**, 121-134 (2000).
12. J. Fleischhauer, U. Höweler, J. Spanget-Larsen, G. Raabe, J. Michl: "Magnetic Circular Dichroism of Nonaromatic Cyclic π -Electron Systems. 5. Biphenylene and Its Aza Analogues", *J. Phys. Chem. A* **108**, 3225-3234 (2004).
13. C. Johannessen, A. Gorski, J. Waluk, J. Spanget-Larsen: "Electronic states of anthanthrene. Linear and magnetic circular dichroism, polarized fluorescence, and quantum chemical calculations", *Polycycl. Arom. Compds.* **25**, 23-45 (2005).
14. D. D. Nguyen, S. V. Hoffmann, N. C. Jones, J. Spanget-Larsen, "Electronic states of model hydrocarbon chromophores investigated by Synchrotron Radiation Linear Dichroism (SRLD) spectroscopy on aligned samples", *ResearchGate* (2010), DOI: [10.13140/RG.2.1.3309.8400](https://doi.org/10.13140/RG.2.1.3309.8400).
15. D. D. Nguyen, N. C. Jones, S. V. Hoffmann, S. H. Andersen, P. W. Thulstrup, J. Spanget-Larsen: "Electronic states of 1,4-bis(phenylethynyl)benzene. A synchrotron radiation linear dichroism investigation", *Chem. Phys.* **392**, 130-135 (2012).

16. P. W. Thulstrup, N. C. Jones, S. V. Hoffmann, J. Spanget-Larsen: “Electronic states of the fluorophore 9,10-bis(phenylethynyl)anthracene (BPEA). A synchrotron radiation linear dichroism investigation”, *Chem. Phys. Lett.* **559**, 35-40 (2013).
17. J. Spanget-Larsen: “LCOAO Computer Program”, PC vs. 2005: Source code with sample input and output, *ResearchGate* (2014), [DOI: 10.13140/2.1.3455.6482](https://doi.org/10.13140/2.1.3455.6482).
18. K. H. Swiatek, J. Spanget-Larsen, “Prediction of UV-VIS Absorbance Data for Polycyclic Aromatic Hydrocarbons (PAHs). Performance of the LCOAO Procedure for Medium to Large Benzenoid Chromophores”, *ResearchGate* (2014), [DOI: 10.13140/2.1.2307.7440](https://doi.org/10.13140/2.1.2307.7440).
19. P. W. Thulstrup, N. C. Jones, S. V. Hoffmann, J. Spanget-Larsen: “UV polarisation spectroscopy of 1,4-diethynylbenzene”, *Mol. Phys.* e1853841 (2020).
20. D. D. Nguyen, N. C. Jones, S. V. Hoffmann, J. Spanget-Larsen: “Near and vacuum UV polarization spectroscopy of 1,4-distyrylbenzene”, *Spectrochim. Acta A* **286**, 122019, pp 1-7 (2023).
21. D. D. Nguyen, N. C. Jones, S. V. Hoffmann, J. Spanget-Larsen, “Excited states of *trans*-stilbene and 1,4-diphenylbutadiene. Near and vacuum UV polarization spectroscopy”, manuscript in preparation.
22. O. Dmytrenko, J. Spanget-Larsen, S. Marzooghi, B. Huyhn, S. Neal, D. Di Toro: “Computational Estimation of Absorbed Photons by Polycyclic Aromatic Hydrocarbons from Polychromatic Sources of Irradiation”, in preparation.