# Quantum Chemistry in the Design of Liquid Crystals for Display Applications

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Since the late 1970s LCDs have grown from Band-Aid size in pocket calculators to ultra-high definition television displays with diagonals of more than one hundred inch. At the same time, the development of liquid crystalline materials for device applications has advanced from relatively simple polar materials (nitriles and esters) to liquid crystals with fluorinated structural elements and fluorinated polar functional groups. The design and optimization of such materials was supported to a large extent by computational quantum chemistry. Pertinent examples for this, such as negative birefringence in calamitic nematic materials, “functional” bridge elements, hypervalent sulfur fluorides, highly polar dielectrically negative indane-derivatives, and the relevance of fluorinated materials to the reliability of LCDs in general will be discussed.