CHIRAL MOLECULAR DESIGN GUIDED BY DATA SCIENCE: [6]HELICENE DERIVATIVES FOR CPL EMISSION

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Chirality is a universal phenomenon, spanning from particle physics to galaxies, but it finds its richest expression at the molecular level. Chiral molecules can absorb or emit circularly polarized light, giving rise to Circular Dichroism (CD) and Circularly Polarized Luminescence (CPL). The ability to emit circularly polarized light is especially attractive for a wide range of applications, including advanced sensing, energy efficiency, and anti-counterfeiting technologies. Designing efficient CPL emitters remains a key challenge, as structure–property relationships are not yet well understood. To address this, we combine quantum chemistry, data science, and genetic algorithms. Thousands of [6]helicene derivatives, a prototypical scaffold, are computed via Density Functional Theory (DFT), extracting key chiroptical parameters. The central quantity is the dissymmetry factor g_{lum}, related to the electric and magnetic transition dipole moments ($\vec{\mu}$ and $\vec{m}$) and their relative orientation θ:

$$g_{\mathrm{lum}} = \frac{4|\vec{m}||\vec{\mu}|\cos\theta}{|\vec{m}|^2 + |\vec{\mu}|^2} \approx \frac{4|\vec{m}|\cos\theta}{|\vec{\mu}|}$$

Machine learning trained on these datasets reveals non-intuitive structural patterns that enhance CPL. Genetic algorithms then guide the design of optimal emitters that can be easily prepared. This synergistic approach transforms molecular design into a physics-guided optimization problem, turning chemical complexity into a data-driven opportunity.

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