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## Rational design of porphyrin and BODIPY analogues for biomedical applications: further progress and future perspectives

Wednesday, 4 December 2024 12:00 (20 minutes)

Over the last two years, considerable further progress has been made in using a rational design approach [1,2] guided by calculations with the Gaussian 09 software package on the Lengau cluster and an application of Michl's perimeter model [3] to prepare novel main group element complexes of porphyrin and boron dipyrromethene (BODIPY) analogues that are suitable for use as photosensitizer dyes in photodynamic therapy against cancer and bacteria [4-8] and as optical limiters in applications relevant to the protection of human eyesight from intense incident laser beams [9-10]. There has been a strong focus on exploring how the lowest energy porphyrin absorption band can be substantially red-shifted into the phototherapeutic window by introducing reduced and confused pyrrole moieties [2,4-7]. Future directions on the use of the Gaussian 09 software package in the context of this research will be described.

### References

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# CHPC Research Programme

## Workshop Duration

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