How can accurate (and not so accurate) calculations be used in spectroscopy?

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Precise computational calculations of electronic structure are essential in spectroscopy. Density Functional Theory is the predominant choice, while ab initio post Hartree-Fock methods, such as multiconfigurational theory[1], remain less explored due to the high computational cost.

This lecture highlights limitations of DFT in accurately describing common spectroscopic phenomena ranging from potential energy surfaces to electronic spectra. Conversely, the multiconfigurational approach offers practical solutions to these challenges [2-4]. Additionally, the lecture thoroughly examines the current limitations and potential applications of multiconfigurational theory in molecular and solid-state spectroscopy, providing insights into the evolving field of computational spectroscopy.

[1] BO Roos, R Lindh, PÅ Malmqvist, V Veryazov, P-O Widmark (2016) "Multiconfigurational Quantum Chemistry", Wiley & Sons.
[2] ED Larsson, M Krosnicki, V Veryazov (2022) Chem. Phys., 562, 111549
[3] ED Larsson, V Veryazov (2023) J Chem Phys, 159, 114117
[4] F Aquilante et al, (2020) J Chem Phys, 152, 214117

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