# Multiconfigurational *ab initio* calculations as a tool to reveal the excited states of transition element impurities in crystals

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In contrast to their high application potential, *e.g.* in wavelength conversion, scintillation or quantum technology, transition elements are notoriously difficult study cases for first principles methods. The incompletely filled *d* (or *f*) shell gives rise to strong electron correlation effects, *i.e.* the electronic states are poorly described by a single Slater determinant. This is however an important requirement to justify the use of single-reference methods such as density-functional theory.
Wave-function-based quantum chemistry is presented as an alternative to study solid state systems. While such methods suffer from the exponential scaling of the wave function, it is shown that insightful and accurate results can nevertheless be obtained by adopting well-considered approximations, in particular by exploiting embedded cluster methods. An additional advantage is that spin-orbit relativistic effects are efficiently incorporated in this methodology, allowing to obtain electronic absorption and emission spectra that can be immediately compared to experiments, also for compounds that contain heavier elements.

[1] Z. Barandiarán, J. Joos, L. Seijo, Luminescent Materials – A Quantum Chemical Approach for Computer-Aided Discovery and Design, Springer, 978-3-030-94983-9 (2022).

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