Title: **Computer assisted design of new [Cr^{II}(R-indenyl)$_2$] molecules with Spin-crossover properties**

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Date: June 2020

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Since its discovery, spin-crossover compounds have attracted attention due to their intrinsic applications as molecular switches. These compounds have two electronic states which can be accessed with similar energies, causing that an external stimulus can determine which one becomes the predominant.

Present work explores the spin-crossover properties of indenyl chromium (II) compound, as some of them exhibit thermally induced spin-crossover transition despite having a rather than unusual metallic centre in the field of spin-crossover properties. To do so, density functional theory and ab initio ligand field theory calculations are performed, with the aim to identify the trends caused by the influence of functionalization of indenyl ligand.

The final goal of the present work is the design of new indenyl chromium (II) compounds with spin-crossover properties and tailored transition temperatures.

Keywords: Spin-crossover, chromium (II), indenyl, density functional theory, DFT, ab initio ligand field theory, AILFT, in-silico design, complexes.