Full energy structure of the Cr^{3+} activator in $Cs_2NaInCl_6$ double halide perovskite host under pressure

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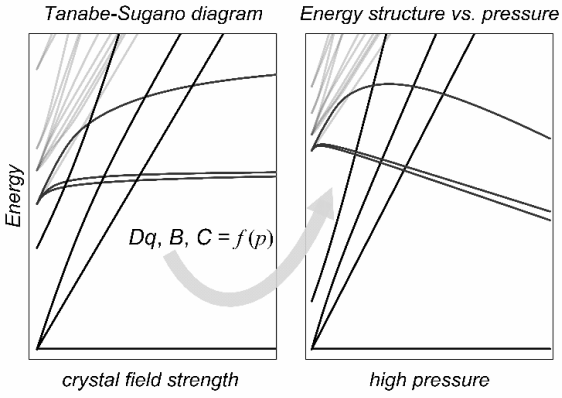
Applying pressure is one of the methods to alter the spectroscopic properties of optical materials activated with transition metal (TM) ions. The energies of electronic transitions of a d^n TM ion are described by an appropriate Tanabe-Sugano (TS) diagram, and the effect of pressure can be superficially understood as increasing the crystal field strength (Dq), i.e. moving right on the TS diagram. The reality is more complex since pressure also affects the mutual electrostatic iteration of the d^n electrons in the TM ion (nephelauxetic effect). This is described by Racah parameters B and C, which can be obtained experimentally.

In this work I report the effect of pressure on radiative transitions in double halide perovskites $Cs_2NaInCl_6$ activated with Cr^{3+} (d^3), by means of high-pressure photoluminescence (PL) and photoluminescence excitation (PLE) spectroscopy. In these materials, a spectacular change between broadband to narrow line emission in the PL spectrum occurs at elevated pressure, resulting from crossover between the $^4T_2$ and ^2E states in the TS diagram.

In this research I am going one step further – utilizing high pressure PLE spectroscopy ton access some of the higher excited states of the system. This allows me to determine all three parameters: crystal field strength Dq, Racah parameters B and C, relevant to the energetic structure of the system. Finally, based on pressure dependence of the parameters, the pressure evolution of all energy levels of the Cr^{3+} dopant is determined, following the approach described in my previous work [1]. In effect an energy diagram of all the crystal field levels of Cr^{3+} dopant in halide perovskite matrix is constructed, which can be understood as the *true* TS diagram of the system, where abstract parameter Dq is replaced by pressure.



[1] Leśniewski T. (2023) Phys. Chem. Chem. Phys., 25, 14449–14462.

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