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ABSTRACT SUBMISSION FORM

Polaronic motion of self-trapped holes in silver halides

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Self-trapped polarons (STPs) are probably the simplest example of defects in solids. They play a key role for explaining the charge transport in many relevant technologies, like organic light emitting diodes or Li-ion batteries. They are also the basis to explain many attractive phenomena like high-temperature superconductivity in the cuprates or colossal magnetoresistance in manganites.

The self-trapped hole (STH) in AgCl, for its relatively simplicity, represents a model system of STP for which it exists a vast amount of experimental data. EPR and ENDOR studies on silver halides started in 1968, proving the formation of a STH in AgCl, but not in AgBr[1]. Laredo et al. showed that STHs in AgCl become mobile above ~35 K, demonstrating the existence of a dominant mechanism of polaronic hopping, involving an activation energy of 61 ± 3 meV[2]. Optical absorption transitions associated with the STH in AgCl peaking at 1.2 eV have been measured experimentally[3]. However, their origin has not been clarified yet.

Here we will try to respond, through a Density Functional Theory model, to some fundamental open questions on small polarons in AgCl and AgBr model systems: (i) What is the equilibrium geometry and the contribution of the local distortion to the binding energy of the STH in AgCl? (ii) How much localized is the STH in the $AgCl_6^{4-}$ complex in AgCl? (iii) Why is the STH stable in AgCl, but not in AgBr? (iv) What is the excitation responsible for the band peaked at 1.2 eV in AgCl? (v) By what mechanisms do the small polarons move through the AgCl lattice?

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