**Nuclear Spin-Induced Circular Dichroism: Using Nuclear Properties to Map Spatial Localization of Excited States**

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Nuclear spin-induced circular dichroism (NSCD) is one of theoretically predicted nuclear magneto-optic effects [1]. NSCD occurs when the electron cloud is excited via a beam of light in the molecule with nuclear spins aligned along the direction of propagation of light. As has been theoretically shown, NSCD arises due to presence of localized interactions, such as paramagnetic spin-orbit coupling $\boldsymbol{h}^{\mathrm{PSO}}$ in the case of non-relativistic theory [1]. Thus, NSCD uniquely combines information about electron excitations with a highly spatially localized properties originating from atomic nuclei. It is of interest to understand how it relates to the molecular structure.

In the presented work we have explored how the spatial localization of the excited states affect the NSCD response of individual nuclei for different excited states [2]. We have used a computational protocol based on quadratic response function, which allows us to look at the NSCD response for different nuclei and each excitation. The results show that a strong NSCD signal for a particular nucleus and excitation can arise only if the nucleus is a part of a chromophore unit that is excited. This finding shows that NSCD could be used as an experimental tool for investigating the location and spatial extent of excited states within molecules.

**References**

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