Journal of Physics: Conference Series **488** (2014) 152001 doi:10.1088/1742-6596/488/15/152001

Matrix effect on the vibronic state of an atom embedded in a Solid Para-H_2

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Synopsis We have examined the matrix effect on the excitation spectra of Xe atom that is embedded in a solid state para-hydrogen $(p\text{-}H_2)_n$ at liquid helium temperature, making use of the ab-initio molecular orbital calculation. The crystal structure of the solid $(p\text{-}H_2)_n$ is hexagonal (hcp) and is known to be a quantum solid that may yield almost free ligand field for an atom located at a lattice point. However, the vibronic states made of $p\text{-}H_2$ molecules coupled with the excited states of Xe atoms, which reflected significant matrix effect on the absorption spectrum in the ultraviolet-visible region. Similar effect on the emission spectra was also studied.

Superradiance (SR) is a cooperative spontaneous emission from an ensemble of emission centers made of atoms or clusters embedded in a solid-state medium [1]. For an ensemble including such centers (number N), the N-dependence of the intensity of coherent radiation and the decay time are proportional to N^2 and $1/N$, respectively. The ordinal SR is due to the single photon emission, whereas we have also investigated the *Paired SuperRadiance* (PSR) due to the two-counterpart photons emitted in opposite directions, i.e., practically no change in the net momentum therein [2]. Although this is an indirect prove, the occurrence of the PSR can identify the neutrino mass.

The *matrix isolation method* using a so-called quantum solid is useful to hold the molecules concerned in a solid as if it was floating, with appropriate density. The solid para-hydrogen ($p\text{-}H_2$) is an ideal matrix for this method, because of less amount of the spectral-shift and more stable trapped-site due to self-annealing of $p\text{-}H_2$, in comparison with other matrixes. Moreover, the solid $(p\text{-}H_2)_n$ can be a candidate that may cause PSR, where high sample density and their long coherence times are plausible [3, 4].

In fact, Kuma et al. has explored the possibility of the PSR for the case of Xe atoms embedded in the solid $(p\text{-}H_2)_n$. They confirmed the presence of the two vibronic states of $v = 1$ and $v = 2$ [5] in the host matrix. When the Xe concentration was about $10^{19}/cm^3$ (0.1 %) in $Xe@(p\text{-}H_2)_n$, they found the significant matrix effect both on the absorption and emission spectra, in the ultra-violet to visible range and infrared range, respectively.

We have evaluated the matrix effect on the excited states of Xe atoms embedded in the hcp crystal of $Xe@(p\text{-}H_2)_n$, making use of ab-initio molecular orbital method. Here, a Xe atom is allocated at the center of a cluster that represents a unit of hcp structure. It is made of twelve ($p\text{-}H_2$) molecules that yields D_{3h} ligand field to the central Xe atom. The spectral shift on the absorption spectra due to the D_{3h} ligand field of solid para-hydrogen was calculated. Further details for the emission spectra will be also presented.

References

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