Investigation of quantum-confined Stark effect on exciton binding energy and electron-hole recombination in GaAs qdots

CHRISTOPHER BLANTON, ARINDAM CHAKRABORTY, Dept. of Chemistry, Syracuse University, Syracuse, NY — We present the field-dependent explicitly correlated full configuration interaction (XCFCI) method for calculating highly accurate electron-hole wavefunction in presence of external electric field. The XCFCI is a variational method which is based on performing FCI calculation using explicitly correlated reference wavefunction. Field-dependent basis functions were used and were constructed using a variational field-dependent coordinate transformation. A discussion between this method and the variational polaron transformation for spin-boson system will be presented. The exciton energy, exciton binding energy (EB), and electron-hole recombination probability (eh-RP) were computed using XCFCI and the analysis of the scaling laws will be presented. One of the key results is that EB and eh-RP follow very different scaling with respect to the field strength. It was found that for a 500 kV/cm change in the field reduces the EB and eh-RP by a factor of 2.6 and 166, respectively. The explicitly correlated term was found to be crucial for accurate computation of eh-RP and was also responsible for improving convergence of the XCFCI energy with respect to basis size. The field dependent basis functions were found to very important and comparison with field independent basis will be presented.

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