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Supporting Information: Theoretical Characterisation of GaSb Colloidal Quantum Dots and their Application to Photocatalytic CO$_2$ Reduction with Water

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Excitonic fine structure

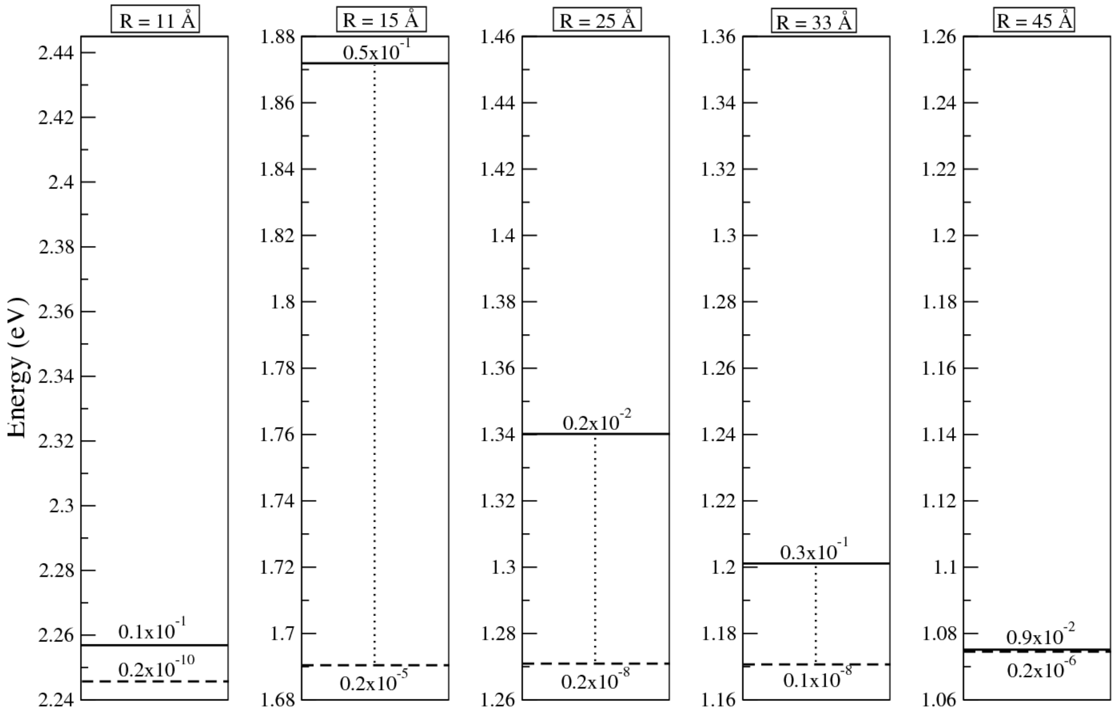

Figure S 1: Ground (dark, dashed lines) and first optically allowed (bright, solid lines) exciton state for different nanocrystal sizes. The calculated value of the CI dipole matrix element (Eq. 2, main text) for the transition $|1e;1h\rangle \rightarrow |0e;0h\rangle$ is also reported for each state. For each size we define as “dark” all excitons with a transition dipole matrix element less than 100 times smaller than that calculated for the strongest optical transition for that size. In the case of $R = 11$ Å the ground exciton is dark and 2-fold degenerate, followed by another 3-fold degenerate dark state 0.32 meV above it and then by the 3-fold degenerate bright exciton. For $R = 45$ Å, there are no other states between the dark, 3-fold degenerate ground state and the 3-fold degenerate bright exciton. In both cases this results in fast radiative recombination times and small Stokes’ shifts. The presence of intermediate states between dark and lowermost bright exciton, found for all other sizes, is marked by vertical dotted lines.