



Deposited via The University of Leeds.

White Rose Research Online URL for this paper:

<https://eprints.whiterose.ac.uk/id/eprint/140928/>

Version: Supplemental Material

Article:

Califano, M and Rodosthenous, P (2018) Theoretical Characterization of GaSb Colloidal Quantum Dots and Their Application to Photocatalytic CO₂ Reduction with Water. *ACS Applied Materials & Interfaces*, 11 (1). pp. 640-646. ISSN: 1944-8244

<https://doi.org/10.1021/acsami.8b15492>

© 2018 American Chemical Society. This document is the unedited Author's version of a Submitted Work that was subsequently accepted for publication in *Applied Materials and Interfaces*, To access the final edited and published work see <https://doi.org/10.1021/acsami.8b15492>

Reuse

Items deposited in White Rose Research Online are protected by copyright, with all rights reserved unless indicated otherwise. They may be downloaded and/or printed for private study, or other acts as permitted by national copyright laws. The publisher or other rights holders may allow further reproduction and re-use of the full text version. This is indicated by the licence information on the White Rose Research Online record for the item.

Takedown

If you consider content in White Rose Research Online to be in breach of UK law, please notify us by emailing eprints@whiterose.ac.uk including the URL of the record and the reason for the withdrawal request.

**Supporting Information: Theoretical
Characterisation of GaSb Colloidal Quantum
Dots and their Application to Photocatalytic CO₂
Reduction with Water**

Marco Califano* and Panagiotis Rodosthenous

*Pollard Institute, School of Electronic and Electrical Engineering, University of Leeds,
Leeds LS2 9JT, United Kingdom*

E-mail: m.califano@leeds.ac.uk

*To whom correspondence should be addressed

Excitonic fine structure

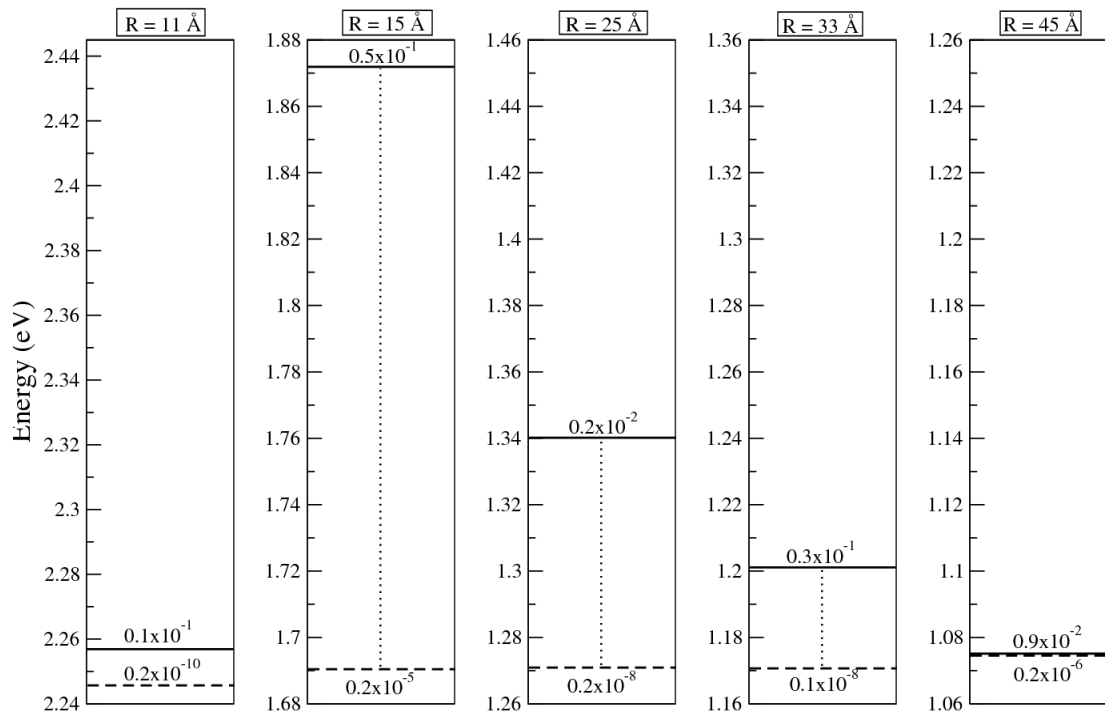


Figure S 1: Ground (dark, dashed lines) and first optically allowed (bright, solid lines) exciton state for different nanocrystal sizes. The calculated value of the CI dipole matrix element (Eq. 2, main text) for the transition $|1e;1h\rangle \rightarrow |0e;0h\rangle$ is also reported for each state. 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.