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Supplementary Information

A simplified theoretical guideline for overall water splitting using photocatalyst particles

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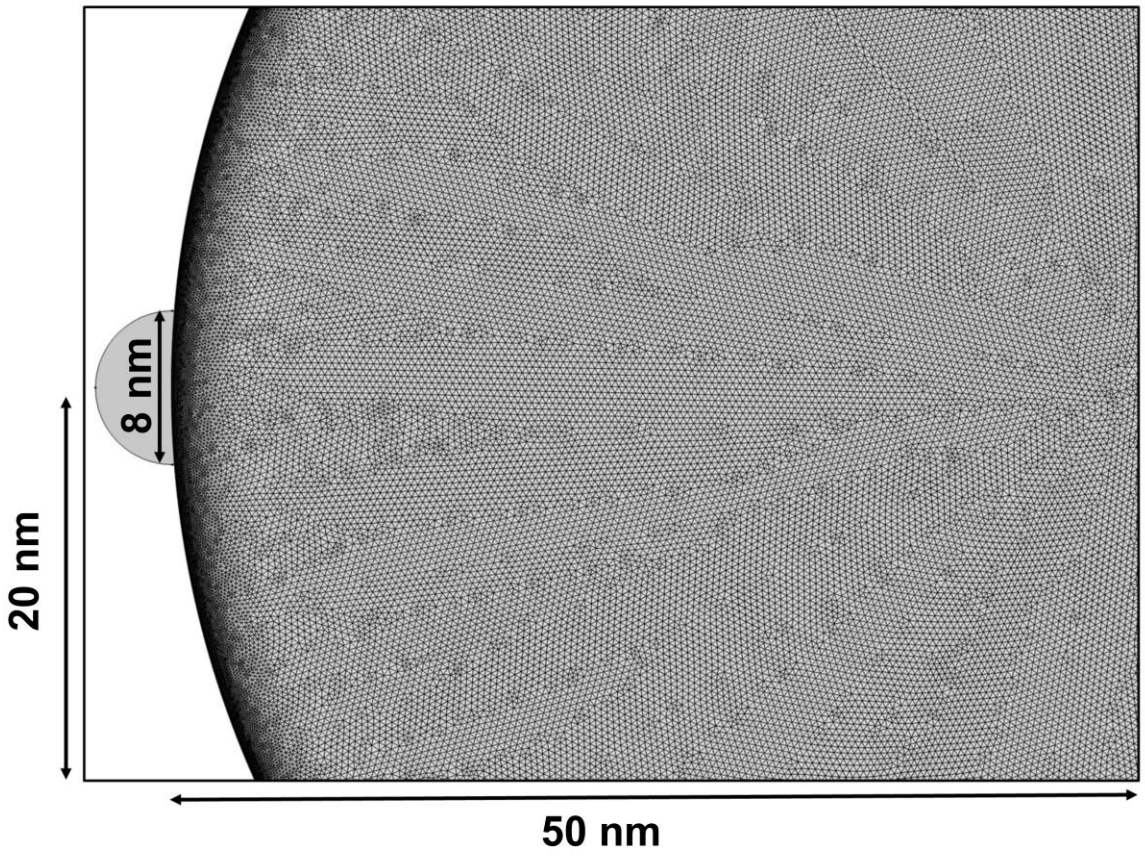

Fig. S1 An example of a typical mesh used for the simulations. The free-triangular mesh was constructed using a minimum element size of 8×10^{-12} m with a growing element rate restricted to a maximum size of 4×10^{-10}.

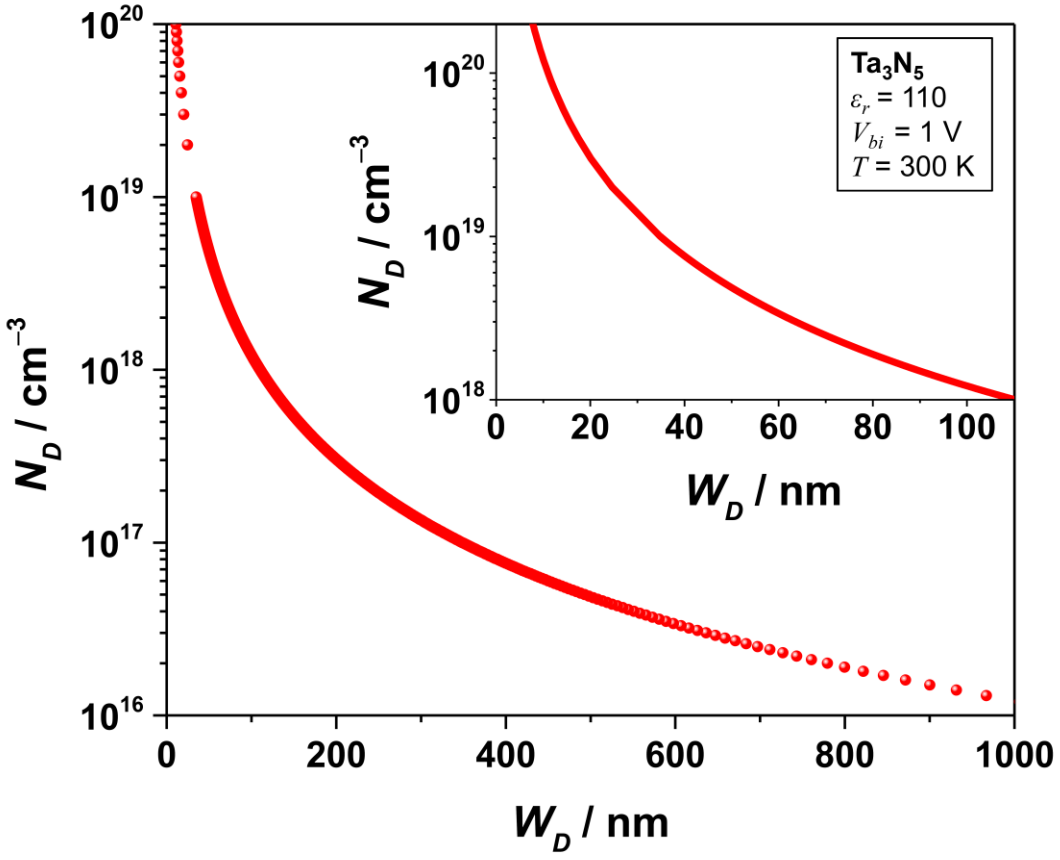

Fig. S2 Solution to Equation 20 assuming a relative dielectric constant of 110 and a built-in potential of 1 V. The consideration of both the electronic and ionic contributions to the calculation of the dielectric constant, resulted in values of >30 but <60 for Ta_3N_5;[1] in the literature, values larger than 100 have been used for this material.[2]

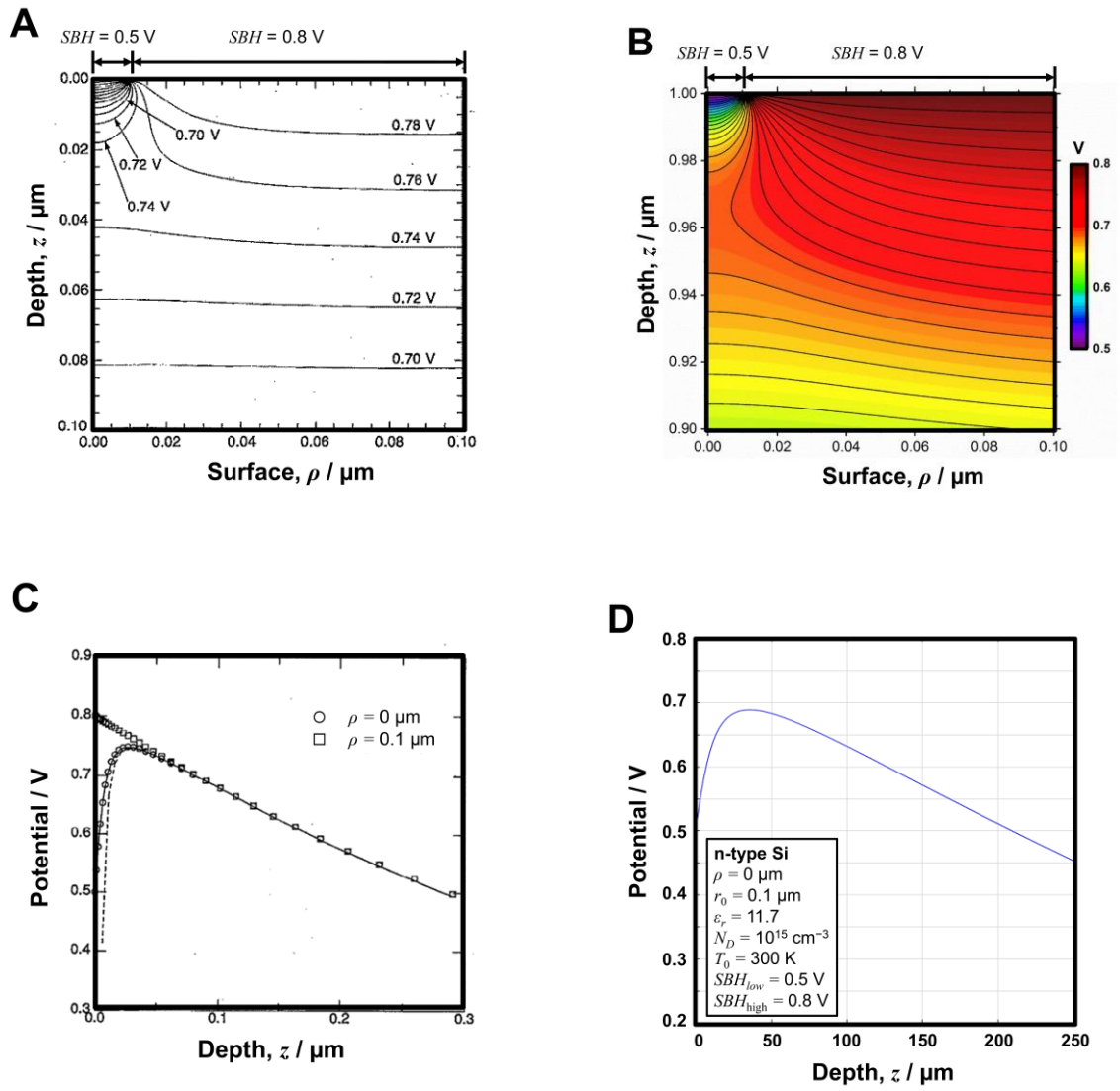

Fig. S3 Equipotential contours obtained from numerical simulations of a polycrystalline *n*-type Si semiconductor at zero applied bias in contact with an inhomogeneous Schottky interface adapted from reference 3 (A and C). Numerical simulations for an *n*-type Si slab with similar geometry and in contact with an interface exhibiting two different Schottky barrier heights as previously proposed in the literature (B and D). The presented results are in reasonable agreement. [3] Similar potential profiles were obtained reproducing the so-called pinch-off effect as observed by Tung et al. (C and D).[4] The potential gradients in the modelled geometry exhibited similar distributions and magnitudes as observed in the Figure (A compared to B and C compared to D). Reprinted with permission from J. P. Sullivan, R. T. Tung, M. R. Pinto, and W. R. Graham, *J. Appl. Phys.*, 1991, 70, 7403. Copyright 1991, AIP Publishing LLC.

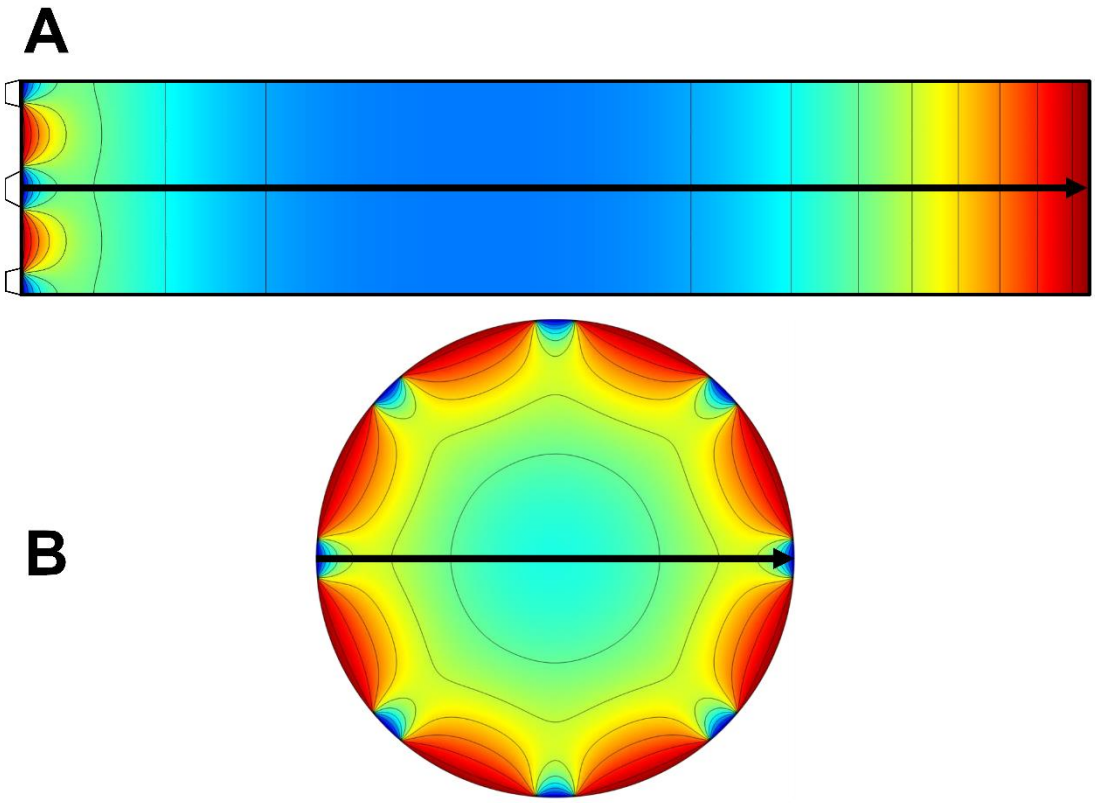

Fig. S4 Cut-lines used to draw the potential profile across the semiconductor model. The objective is to illustrate the one-dimensional energy profile across the material from one interface to the other. The cut-line was made under the catalyst in Ohmic contact towards the opposite electrolyte interface forming a rectifying junction (A). The potential was drawn starting at the metal site forming an Ohmic contact, into the semiconductor hemispherical particle, towards another Ohmic interface on the opposite interface (B).

References

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3 J. P. Sullivan, R. T. Tung, M. R. Pinto, and W. R. Graham, *J. Appl. Phys.*, 1991, **70**, 7403.

4 R. T. Tung, *Appl. Phys. Lett.*, 1991, **58**, 2821.