Supporting Information for: Decoupling Radiative and Auger Processes in Semiconductor Nanocrystals by Shape Engineering

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AC times as a function of arm length and TP volume

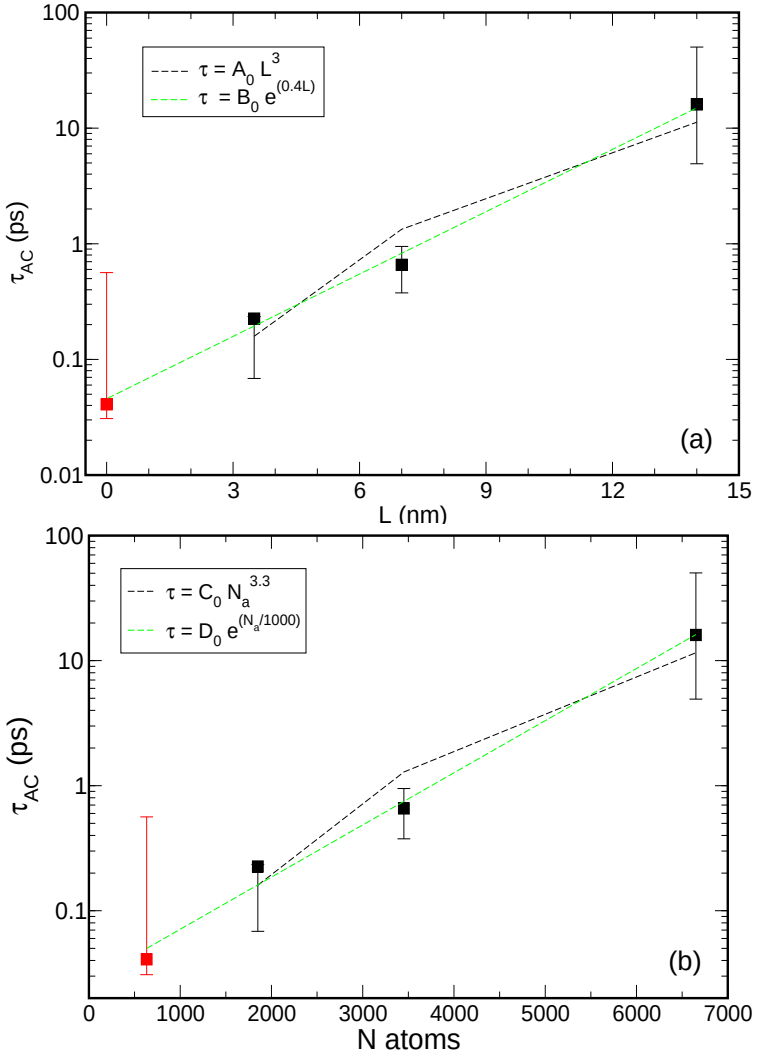

Figure S 1: Auger cooling (AC) relaxation times in CdTe TPs with $D = 2.1$ nm, calculated as a function of L (a) and as a function of the volume (b), expressed as the total number of atoms in the TP, N_a. Black and green dashed lines, indicate fits to power (ax^p) and exponential (be^{cx}) functions, respectively. We find $A_0 = 3.4 \times 10^{-3}$, $B_0 = 4.6 \times 10^{-2}$, $C_0 = 1.8 \times 10^{-12}$, and $D_0 = 2.7 \times 10^{-2}$ give the best fits. The red symbol represents the AC lifetime calculated for a CdTe quantum dot with $R = 1.7$ nm for reference.

AR times as a function of TP volume

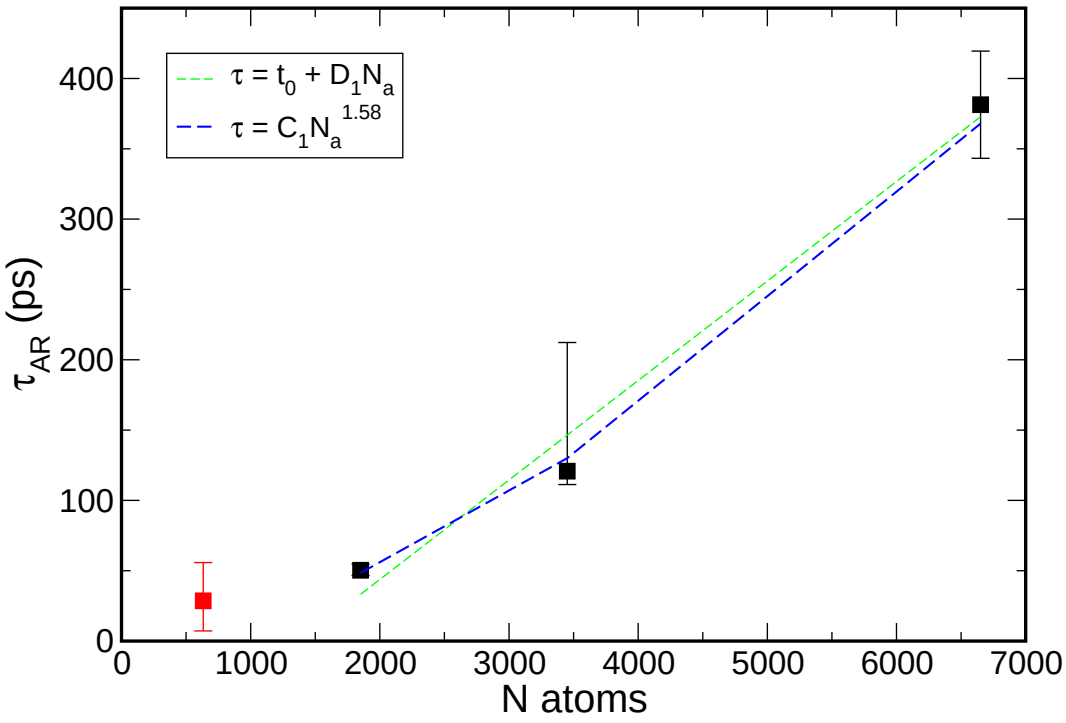

Figure S 2: Auger recombination (AR) times in CdTe TPs with $D = 2.1$ nm, calculated as a function of the TP volume, expressed as the total number of atoms in the TP, N_a. Blue and green dashed lines, indicate fits to power ($C_1 x^p$) and linear ($t_0 + D_1 x$) functions, respectively. We find $C_1 = 3.2 \times 10^{-4}$, $p = 1.58$, $t_0 = -97.7$ $D_1 = 7 \times 10^{-2}$ give the best fits. The red symbol represents the AC lifetime calculated for a CdTe quantum dot with $R = 1.7$ nm for reference.

Auger Cooling: comparison of the lifetimes calculated using two different approaches for the screening

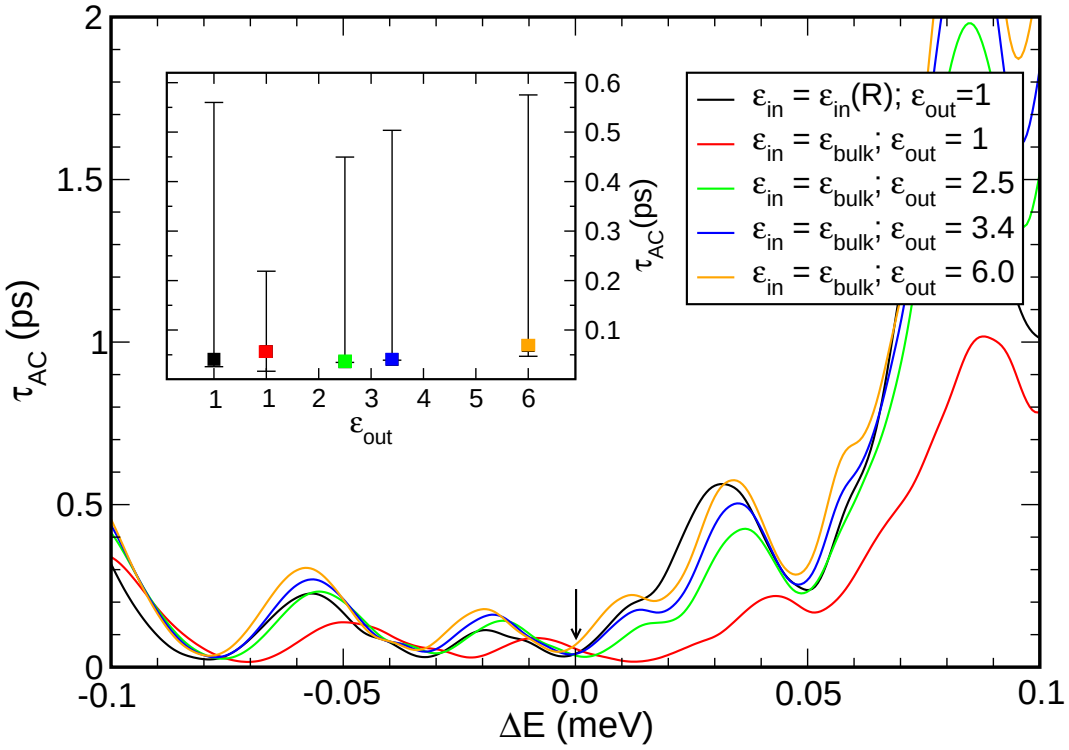

Figure S 3: Comparison of the Auger Cooling lifetimes calculated, as a function of the energy variation around the calculated electron transition energy (corresponding to $\Delta E = 0$), in a CdTe spherical nanocrystal with $r = 1.7$ nm, using the 'regional screening' approach of Wang *et al.*[1] (coloured lines and symbols), and the 'size-dependent screening' approach of Franceschetti *et al.*[2] (black line and symbols). In the 'regional screening' approach the dielectric constant inside the dot (ϵ_{in}) is assumed equal to the bulk dielectric constant. The variation to the external dielectric constant ϵ_{out} occurs via a smoothly decaying sine-like function.[1] The 'size-dependent screening' approach assumes ϵ_{in} to be size- and position-dependent[2] and $\epsilon_{out} = 1$.

Auger Recombination: comparison of the lifetimes calculated using two different approaches for the screening

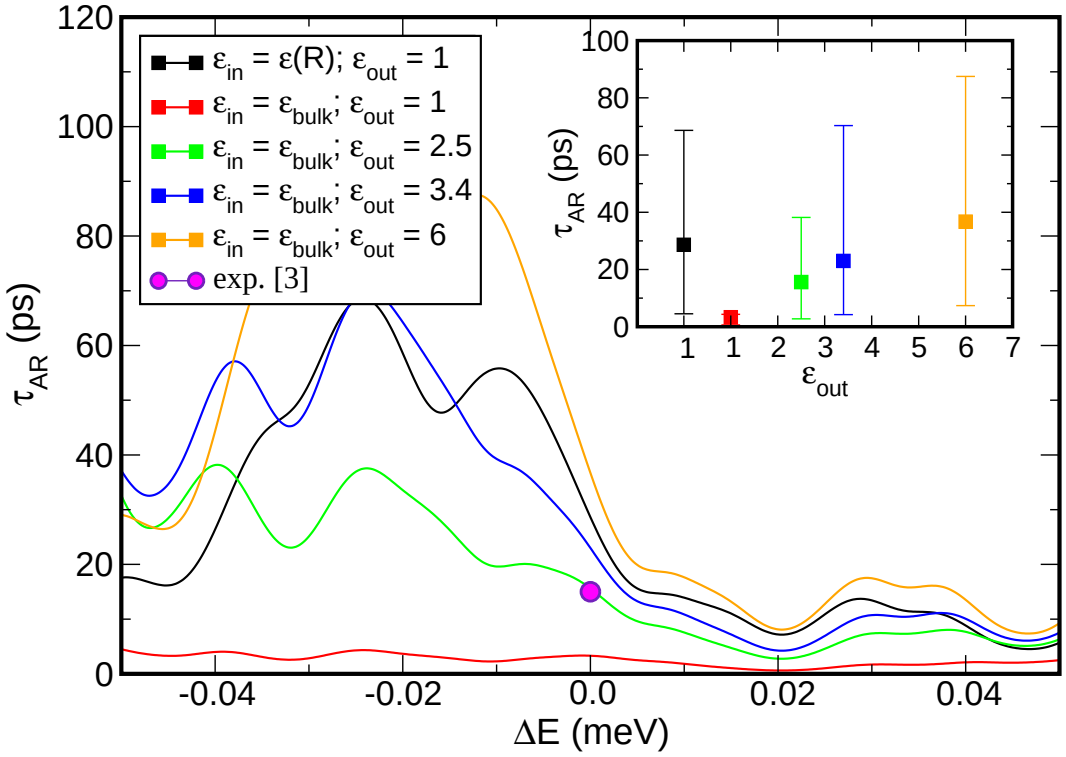

Figure S 4: Comparison of the Auger Recombination lifetimes calculated, as a function of the energy variation around the calculated single-particle gap (corresponding to $\Delta E = 0$), in a CdTe spherical nanocrystal with $r = 1.7$ nm, using the 'regional screening' approach of Wang *et al.*[1] (coloured lines and symbols), and the 'size-dependent screening' approach of Franceschetti *et al.*[2] (black line and symbols). Experimental data relative to a CdTe spherical dot with $D = 3.4$ nm (magenta circle)[3] are also included for comparison. In the 'regional screening' approach the dielectric constant inside the dot (ϵ_{in}) is assumed equal to the bulk dielectric constant. The variation to the external dielectric constant ϵ_{out} occurs via a smoothly decaying sine-like function.[1] The 'size-dependent screening' approach assumes ϵ_{in} to be size- and position-dependent[2] and $\epsilon_{out} = 1$.

References

(1) Wang, L.-W.; Califano, M.; Zunger, A.; Franceschetti, A. Pseudopotential Theory of Auger Processes in CdSe Quantum Dots. *Phys. Rev. Lett.* **2003** *91*, 056404.

(2) Franceschetti, A.; Fu, H.; Wang, L.-W. & Zunger, A. Many-Body Pseudopotential Theory of Excitons in InP and CdSe Quantum Dots. *Phys. Rev. B* **1999**, *60*, 1819-1829.

(3) Kobayashi, Y.; Pan, L.; Tamai, N. Effects of Size and Capping Reagents on Biexciton Auger Recombination Dynamics of CdTe Quantum Dots. *J. Phys. Chem. C* **2009**, *113*, 11783-11789.