Supporting Information: Charge Dynamics in Quantum-Dot-Acceptor Complexes in the Presence of Confining and Deconfining Ligands

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Comparison between the charge densities calculated for hole-deconfining (HD) and hole-non-deconfining (HND) linkers

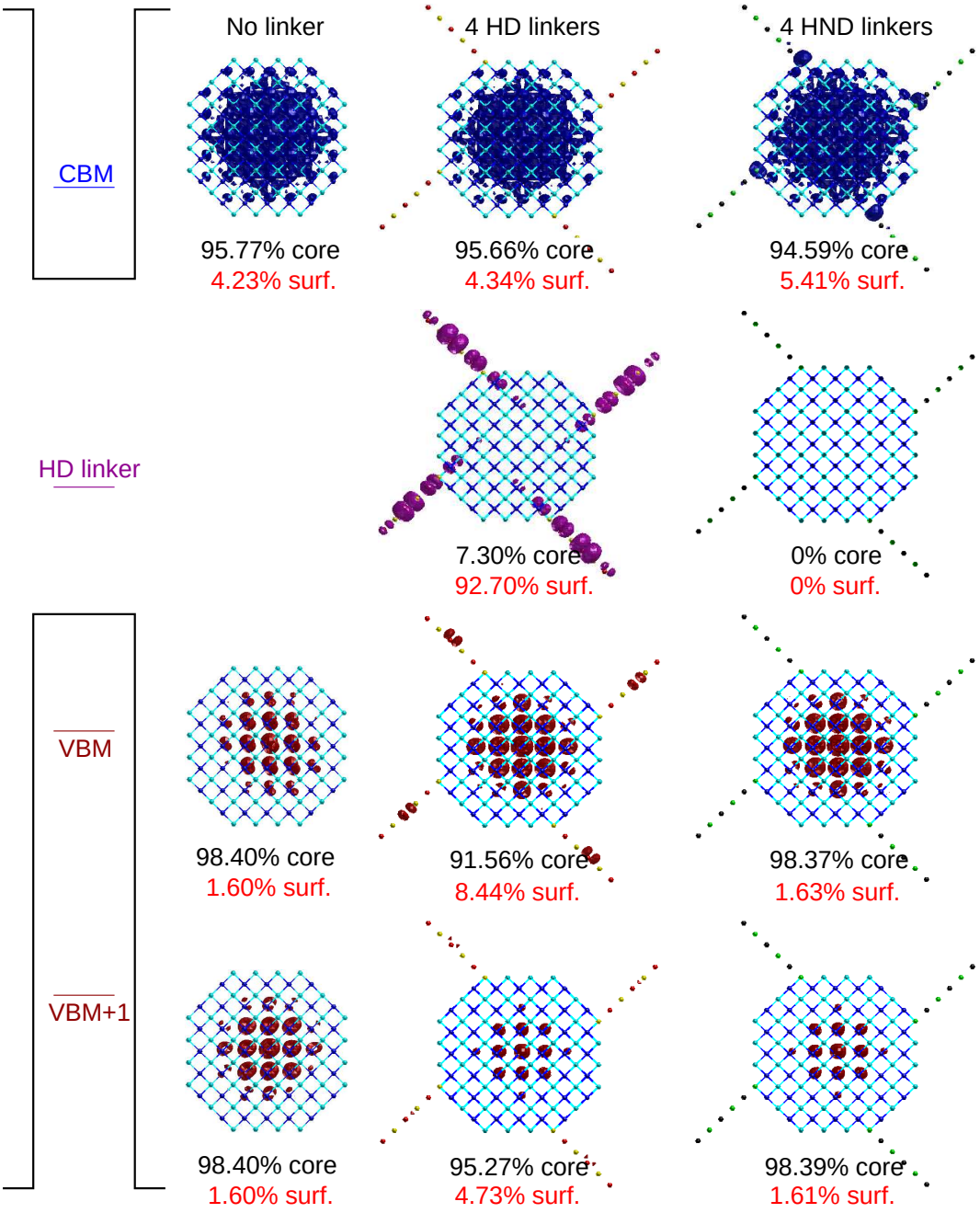

Figure S 1: Comparison of the calculated charge density distribution for cbm (blue, upper panels), linker states (magenta, middle panels), and vbm and vbm+1 (red, lower panels), in the case of a bare NC (left), and in the presence of 4 HD linkers (center), and 4 HND linkers (right). All charge densities are shown superimposed onto the atomic structure of NC and linker, together with the percentage of localization within the dot core (black figures) and on the surface (red figures). Although the number of linker states in the gap equals the number of ligands on the surface, the charge density of only one representative linker state is shown. A cartoon of the electronic structure showing the relevant energy level (not to scale) is also shown on the left.

Calculated Auger-mediated hole transfer times in a CdSe NC with four PTC/PTZ conjugates

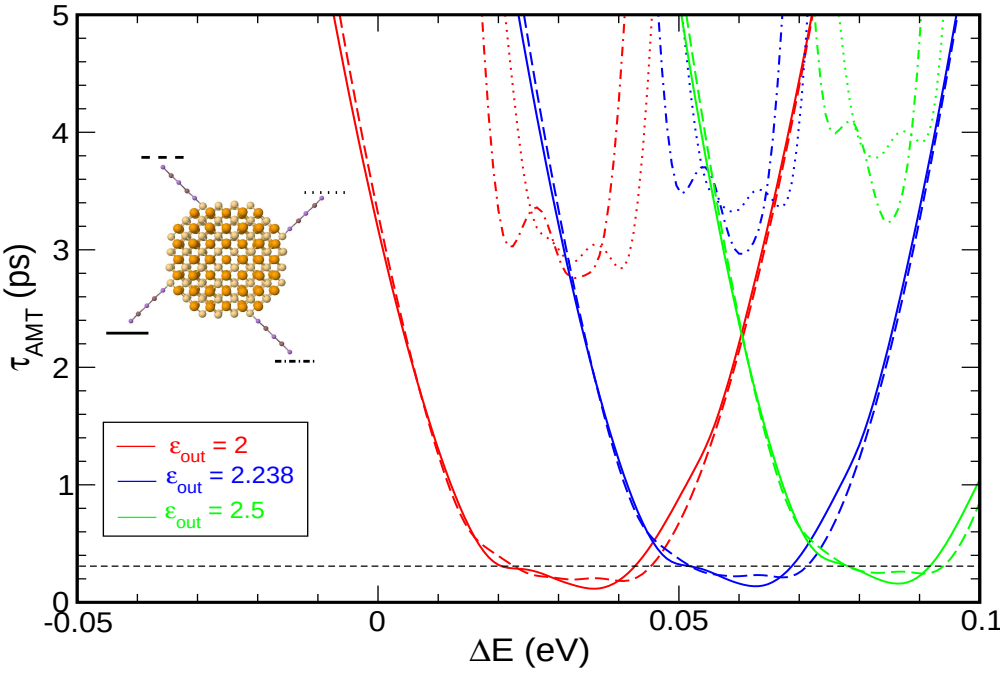

Figure S 2: Auger-mediated hole transfer times in a CdSe NC with four linker-acceptor (m-PTC/m-PTZ) complexes, calculated as a function of the variation of the energy position of the linker-acceptor HOMO with respect to its calculated value (-5.44 eV, $\Delta E = 0$), for different values of the dielectric constant of the NC-acceptor conjugate's environment, from 2 (red curve) to 2.5 (green curve), covering common ligands and solvents. Solid, dashed, dotted and dash-dotted lines refer to linker-acceptor located, respectively, on the bottom left, top left, top right, and bottom right of the NC, as shown in the cartoon.

Charge density in the presence of an electron-non-deconfining (END) linker

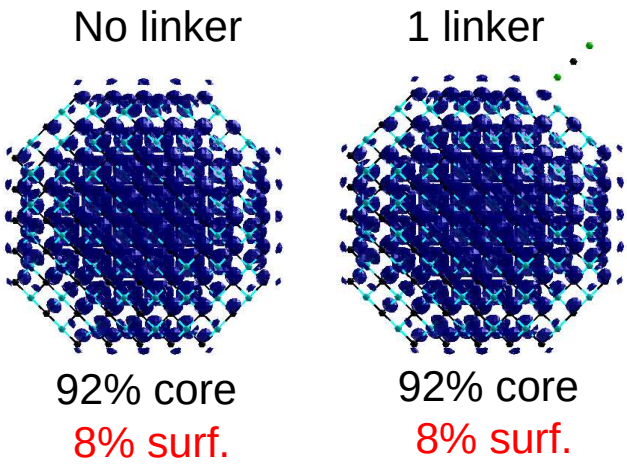

Figure S 3: Comparison between the CBM charge density calculated for a bare NC and in the presence of an END linker. All charge densities are shown superimposed onto the atomic structure of NC and linker, together with the percentage of localization within the dot core (black figures) and on the surface (red figures). No states in the gap nor hybrid ligand-CB states are found in this case.

AMeT times from a core electron

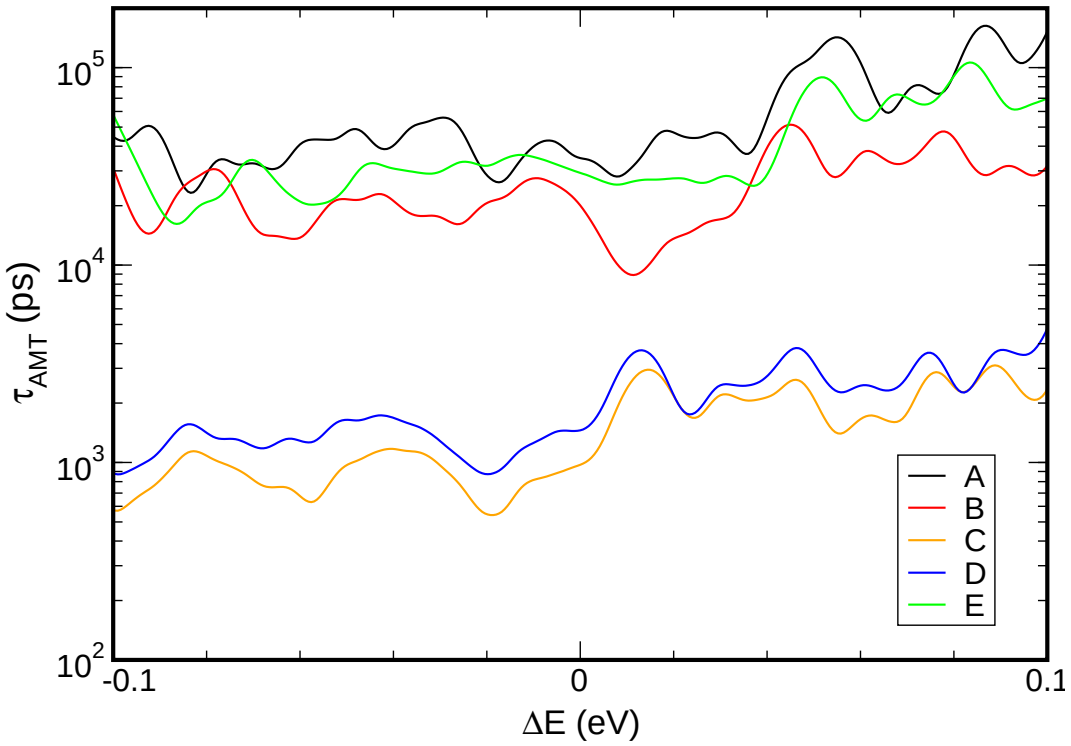

Figure S 4: Auger-mediated electron transfer times from a core (CBM) electron to a single linker-acceptor complex, calculated as a function of the variation of their energy separation ΔE with respect to its calculated value ($\Delta E = 0$), for different combinations (A-E) of the linker position on the NC surface and of the acceptor on the linker end group. The value of the dielectric constant of the NC-acceptor conjugate's environment is 2.238.

AMeT times from a surface-trapped electron

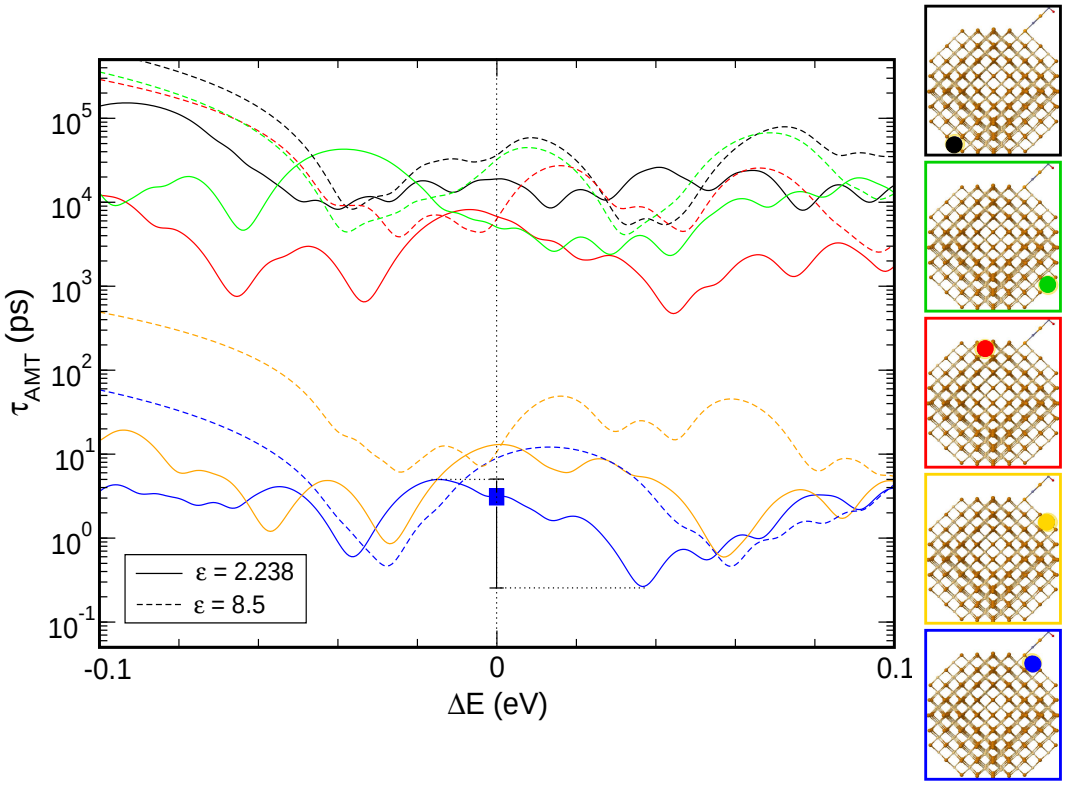

Figure S 5: Auger-mediated electron transfer times from a surface trap to a single linker-acceptor complex, calculated as a function of the variation of their energy separation ΔE with respect to its calculated value ($\Delta E = 0$), for different values of the dielectric constant of the NC-acceptor conjugate's environment, from 2.238 (solid lines) to 8.5 (dashed lines). AMT times are reported for 5 different locations of the trap on the NC surface, indicated by the colored spheres (color coded with the lines in the graph) in the atomistic structure cartoons on the right (the spheres' dimensions are exaggerated for clarity). The data in Fig. 5 of the main text are obtained as shown by the blue square with error bars in the lowermost part of the graph.