Weak spots in semiconductor nanoplatelets: from isolated defects towards directed nanoscale assemblies

Supporting Information

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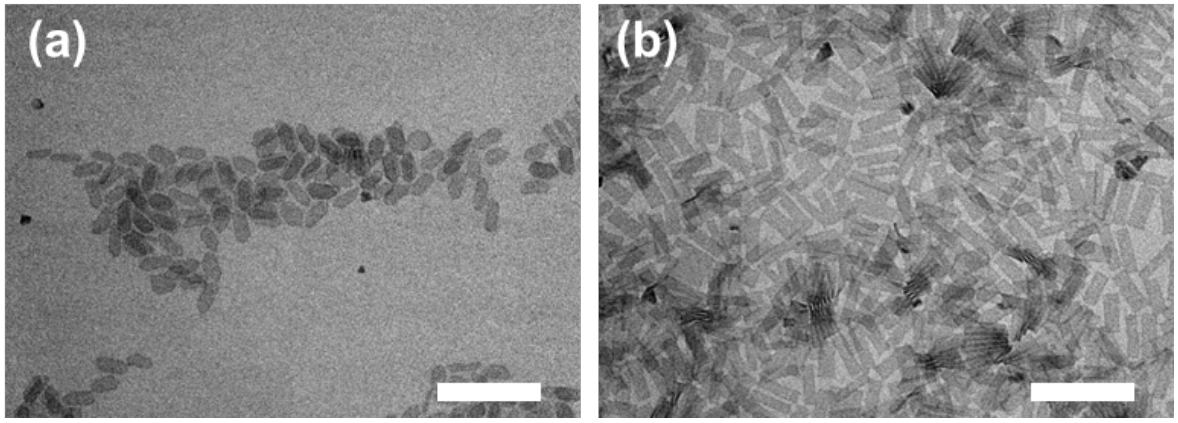

Figure S1 Bright field TEM analysis of CdSe NPLs (a) before, and (b) after seeded growth. All scalebars are 100 nm.

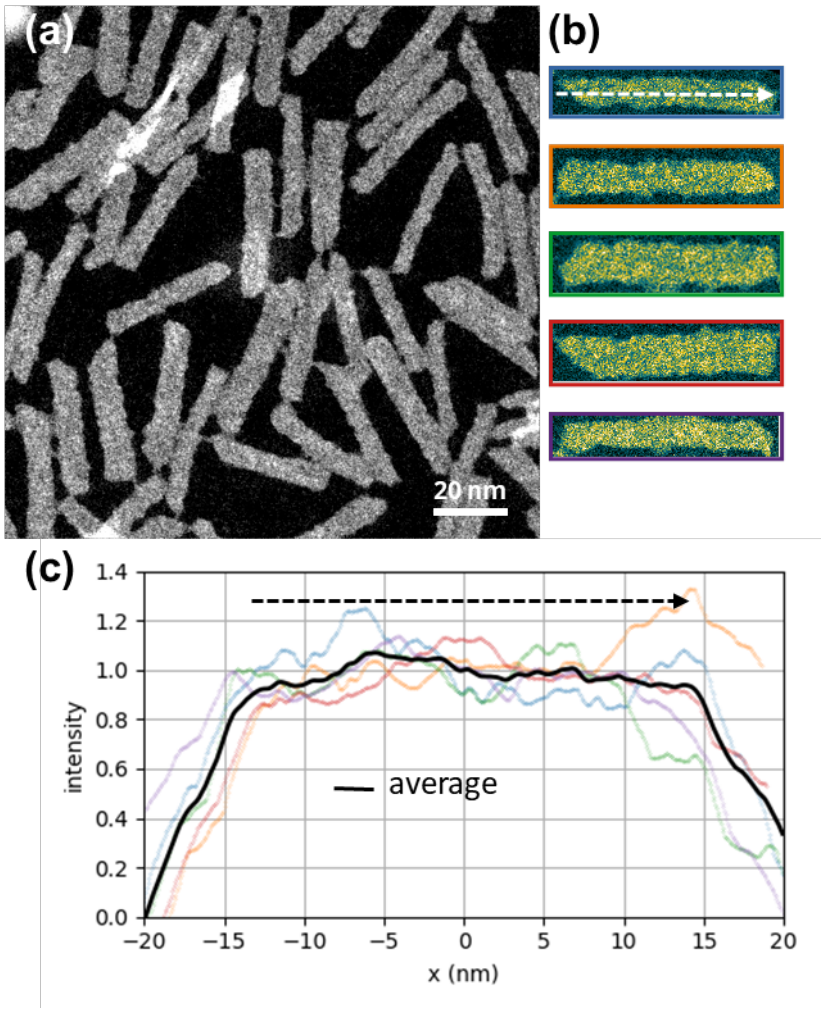

Figure S2 TEM analysis of $Cd_{0.98}Hg_{0.02}Se$ nanoplatelets. (a) HAADF STEM overview image, (b) HAADF STEM of selected nanoplatelets. (c) Intensity at long axis of nanoplatelets, transformed to common size.

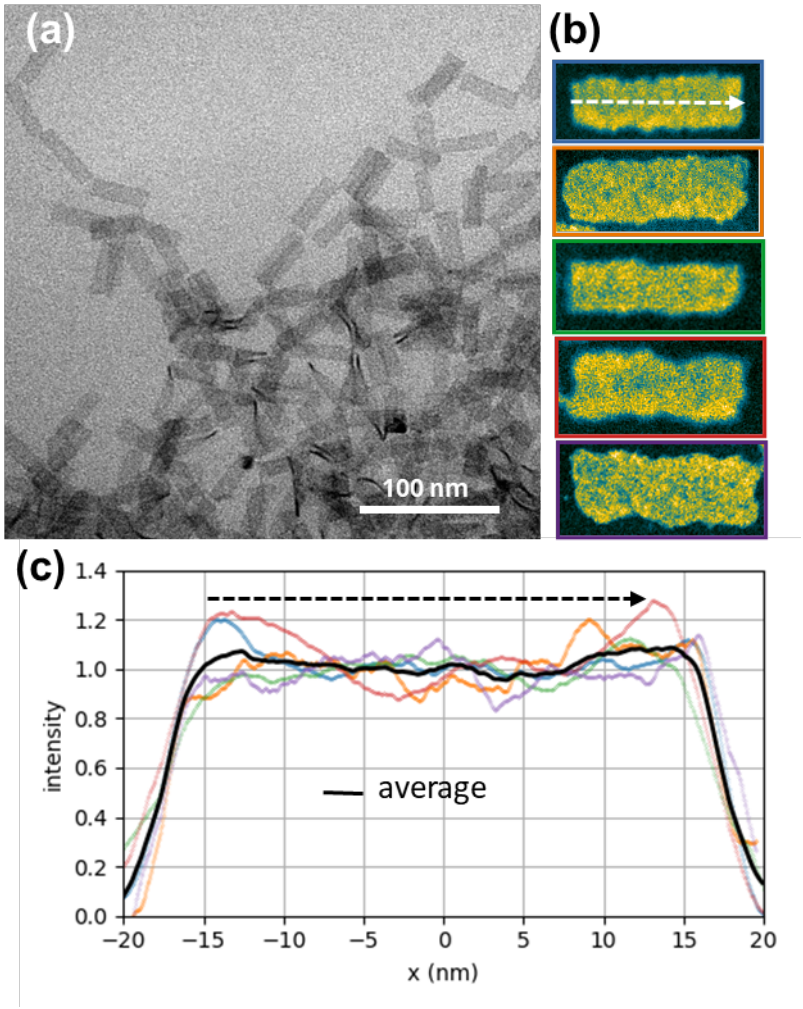

Figure S3 TEM analysis of $Cd_{0.95}Hg_{0.05}Se$ nanoplatelets. (a) TEM overview image (b) HAADF STEM of selected nanoplatelets. (c) Intensity at long axis of nanoplatelets, transformed to common size.

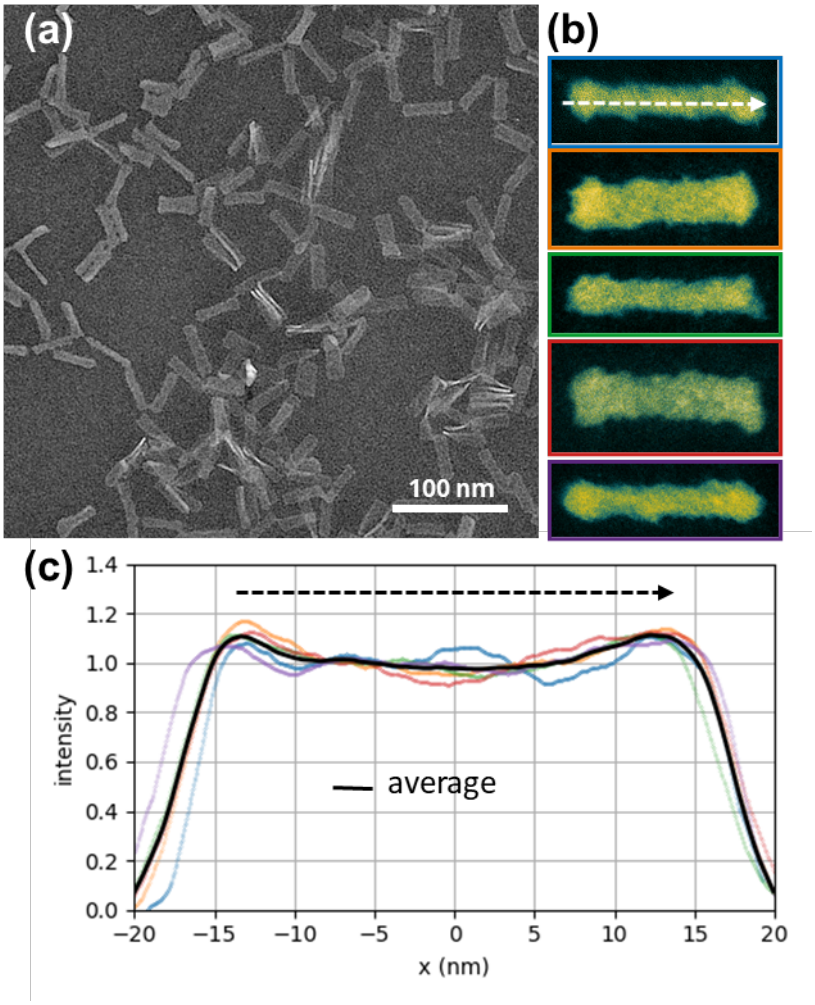

Figure S4 TEM analysis of $Cd_{0.9}Hg_{0.1}Se$ nanoplatelets. (a) TEM overview image (inverted colour), (b) HAADF STEM of selected nanoplatelets. (c) Intensity at long axis of nanoplatelets, transformed to common size.

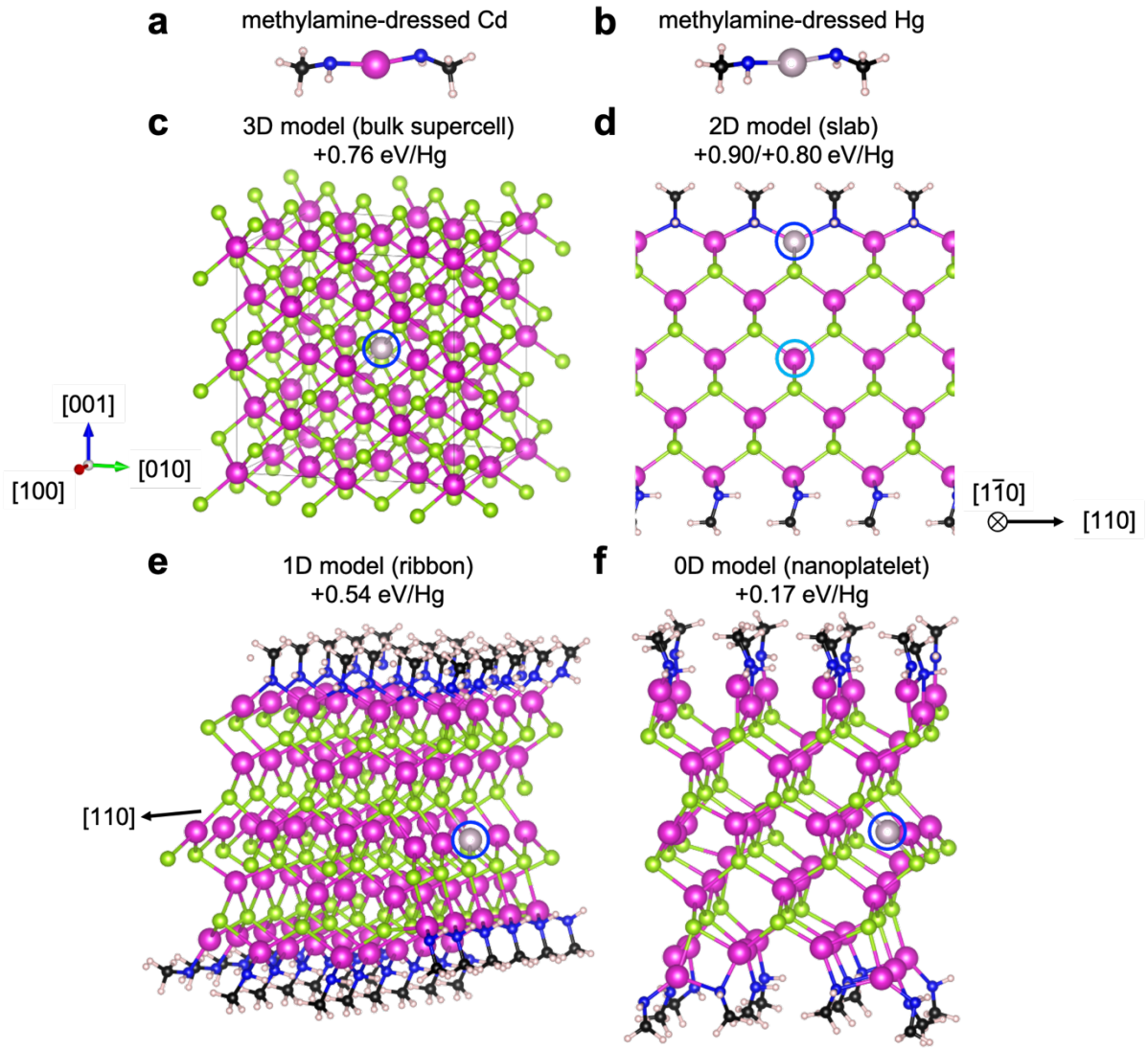

Figure S5 Cation exchange with methylamine ligands. The methylamine-dressed cations of Cd (a) and Hg (b). Hg substitution in (c) a 3D model (bulk 2×2×2 supercell), (d) a 2D model (slab with (001) surfaces), (e) a 1D model (ribbon), and (f) a 0D model (nanoplatelet). The respective substitution energies are also indicated. The substituting Hg ions are surrounded by a dark blue circle. In case of the 2D slab, also the energy for substituting the central Cd marked by the light blue circle was calculated. Colours: Cd magenta, Se green, Hg gray, C black, N blue, and H off-white.

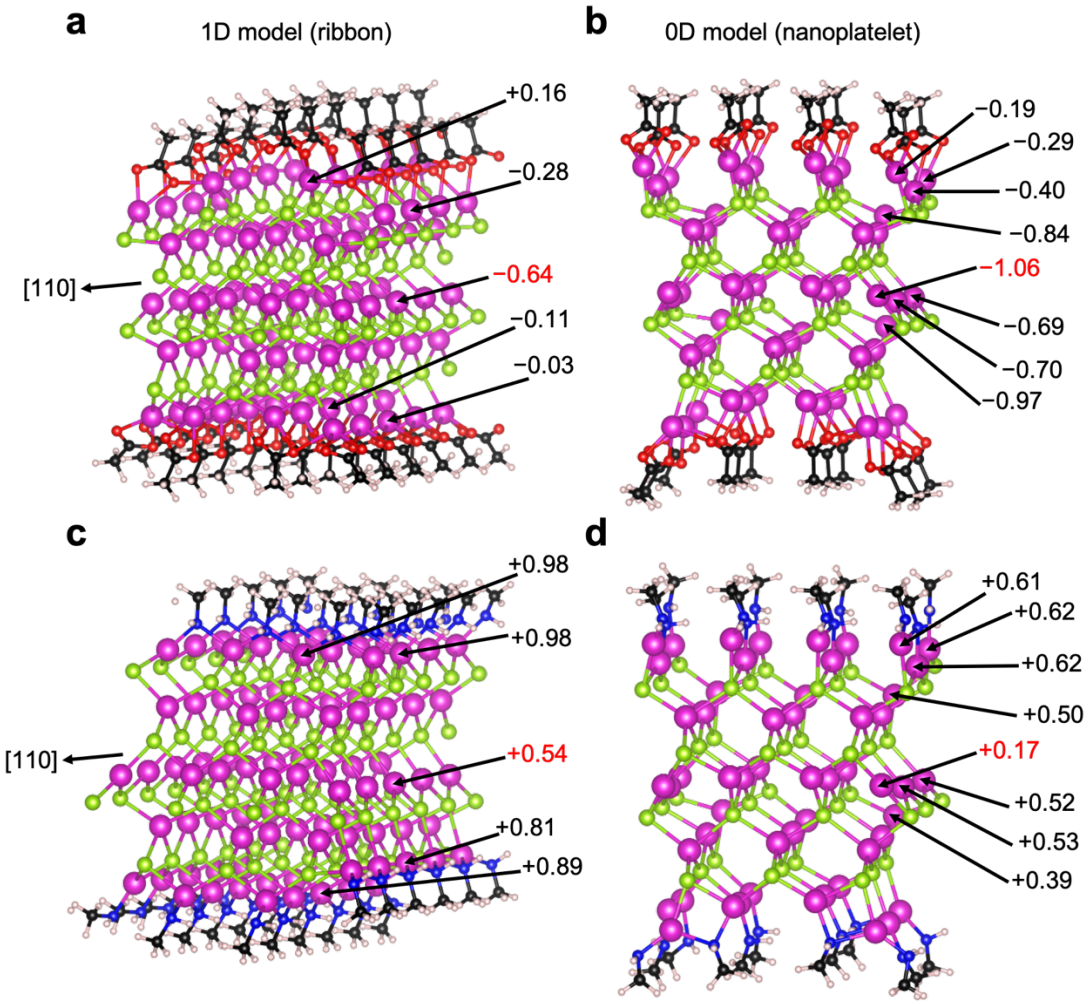

Figure S6 Cation exchange at different ribbon and platelet sites. Indication of the different substitution sites investigated for the 1D model (ribbon) (a, c) and the 0D model (nanoplatelet) (b, d) for acetate or methylamine ligands at the surface, respectively. In each case, the site is labelled by the substitution energy per Hg. The lowest number representing the largest energy gain (or smallest energy loss in case of positive values) upon cation exchange is indicated in red in each case.