Supporting Information for

A Generalized Ligand-Exchange Strategy Enabling Sequential Surface Functionalization of Colloidal Nanocrystals

Angang Dong,†,† Xingchen Ye,† Jun Chen,‡ Yijin Kang,† Thomas Gordon,† James M. Kikkawa,§ and Christopher B. Murray†,‡

†Department of Chemistry, ‡Department of Materials Science and Engineering, §Department of Physics & Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, †The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California 94720

Figure S1. (A and B) Low- and high-magnification TEM images of NOBF₄-treated PbS NCs (~ 10 nm) dispersed in DMF, respectively, showing the aggregation of NCs after surface treatment. (C and D) Low- and high-magnification TEM images of NOBF₄-treated PbTe NCs (~ 6 nm) dispersed in DMF, respectively, showing the fusion of NCs after surface treatment.
**Figure S2.** Comparison of FTIR spectra of OA molecules and molecular species stripped from the NC surface, which were retrieved by drying the supernatant after NOBF₄ treatment.
**Figure S3.** ζ-potential measured for the BF$_4^-$-modified NCs dispersed in DMF: (A) Fe$_3$O$_4$ NCs (10 nm), (B) TiO$_2$ nanorods (~ 3 nm × 20 nm), (C) FePt NCs (4 nm).
Figure S4. FTIR spectra of CoPt$_3$ NCs before and after treatment with 4-bromobenzenediazonium tetrafluoroborate, respectively, showing the presence of BF$_4^-$ anions and DMF molecules at the NC surface upon surface modification.
Figure S5. Comparison of upconversion emission spectra of NaYF₄:Yb/Er nanorods (~30 nm × 50 nm) before (dispersed in hexane) and after (dispersed in DMF) NOBF₄ treatment, showing essentially identical emission intensity. The inset shows the TEM images of the nanorods dispersed in DMF.
Figure S6. Cyclic voltammograms of Fe$_{0.5}$Pt$_{0.5}$ NCs (4 nm) treated with TMAOH, and NOBF$_4$, respectively.
Figure S7. FTIR spectra of FePt NCs capped by various ligands which are obtained by a secondary ligand-exchange process.
Figure S8. H$_2$O-soluble NCs obtained by functionalizing the BF$_4$-modified NCs with PVP. TEM image (A) and DLS measurement (B) of the PVP-functionalized Fe$_3$O$_4$ NCs (10 nm) dispersed in H$_2$O, confirming the aggregate-free nature of the colloidal dispersion. (C) TEM image of the PVP-functionalized FePt NCs (4 nm) dispersed in H$_2$O. The insets in (A) and (C) show the photographs of the corresponding NCs dispersed in H$_2$O. The upper layer is hexane.