**SUPPORTING INFORMATION**

# Phase-Selective Solution Synthesis of Perovskite-Related Cesium Cadmium Chloride Nanoparticles

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| Material | Exp. *a* (Å) | PBE *a* (Å) | HSE06 *a* (Å) | Exp. *c* (Å) | PBE *c* (Å) | HSE06 *c* (Å) |
|---|---|---|---|---|---|---|
| $CsCdCl_3$ | 7.58 | 7.57 | 7.52 | 18.87 | 18.86 | 18.70 |
| $Cs_2CdCl_4$ | 5.26 | 5.38 | 5.34 | 16.88 | 17.11 | 17.01 |
| $Cs_3Cd_2Cl_7$ | 5.24 | 5.37 | 5.32 | 27.24 | 27.67 | 27.51 |

**Table S1.** Experimental and computational lattice parameters.

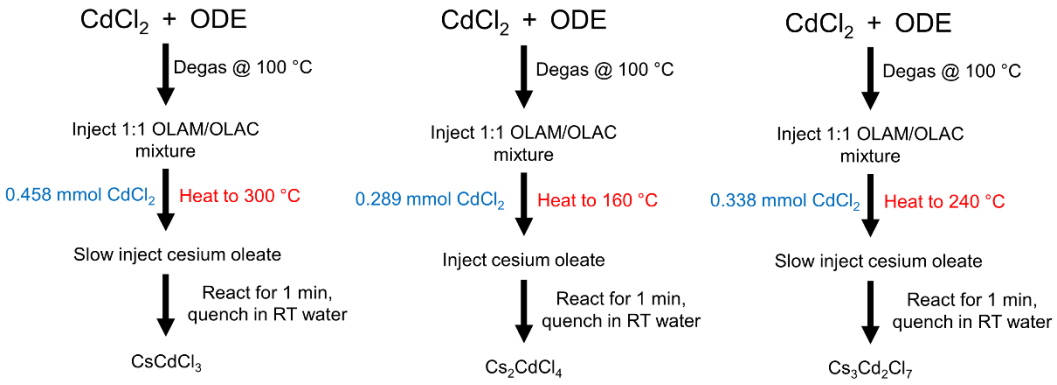


**Figure S1**. Reaction schemes for the solution synthesis of $CsCdCl_3$, $Cs_2CdCl_4$, and $Cs_3Cd_2Cl_7$ particles.

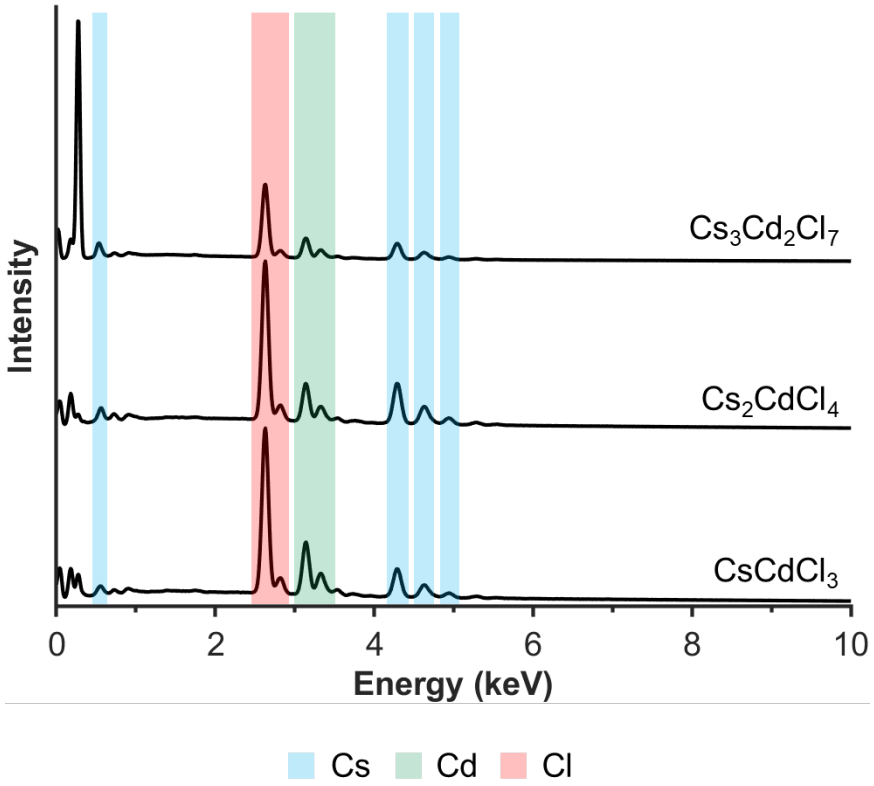


**Figure S2.** EDS spectra for $CsCdCl_3$, $Cs_2CdCl_4$, and $Cs_3Cd_2Cl_7$ nanoparticles.

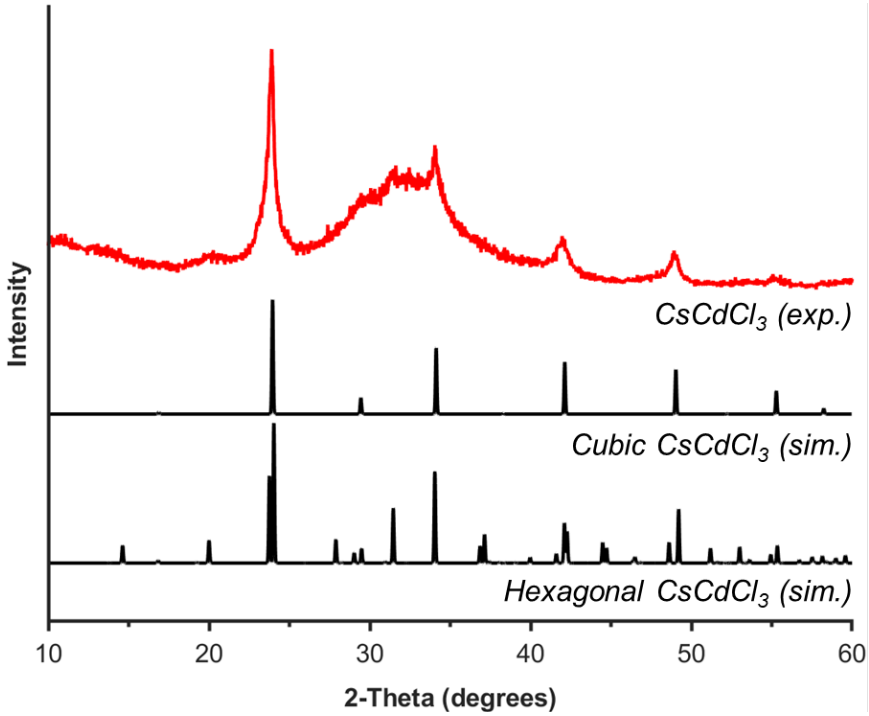


**Figure S3.** Experimental XRD pattern showing a mixture of the cubic and hexagonal $CsCdCl_3$ phases when slowly injecting cesium oleate at lower temperatures. The simulated reference patterns are also presented on the bottom.

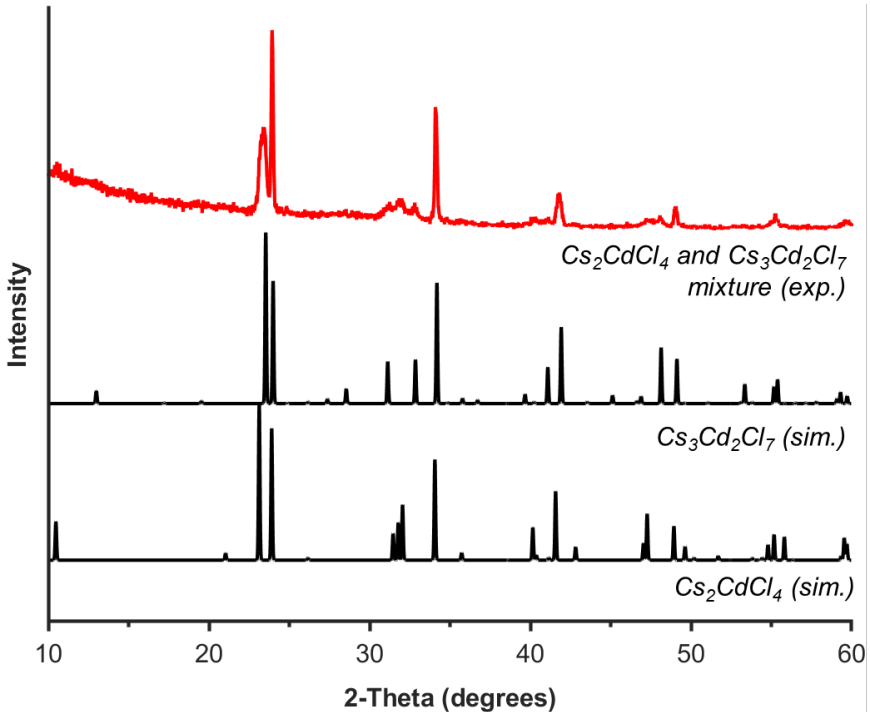


**Figure S4.** Experimental XRD pattern showing a mixture of $Cs_3Cd_2Cl_7$ and $Cs_2CdCl_4$ after injecting the cesium oleate solution swiftly at 240 °C. The simulated references patterns are also shown on the bottom.

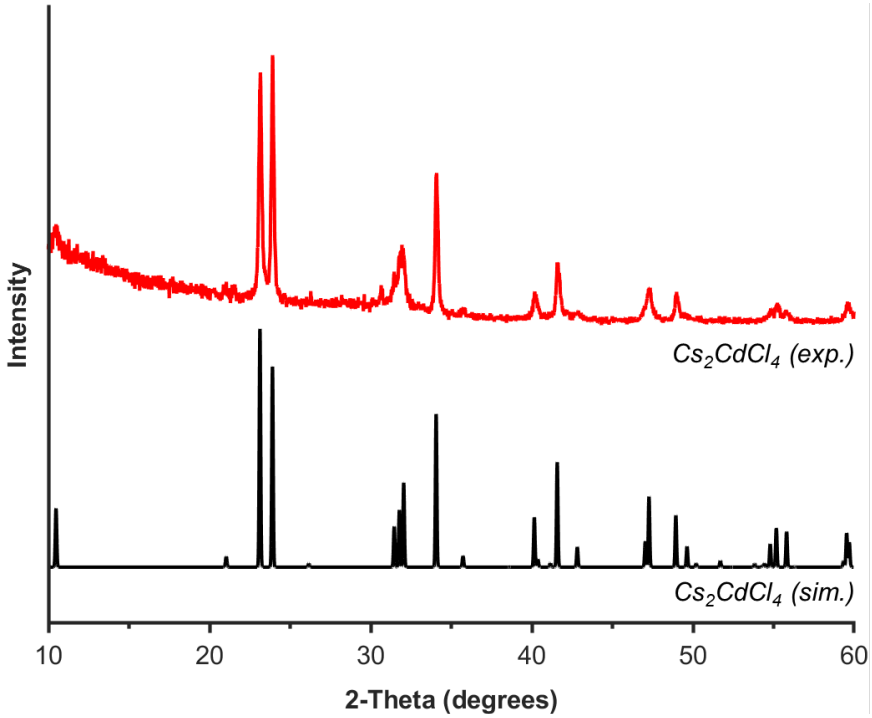


**Figure S5.** Experimental and simulated XRD pattern showing nearly phase-pure $Cs_2CdCl_4$ after injecting swiftly at 160 °C.

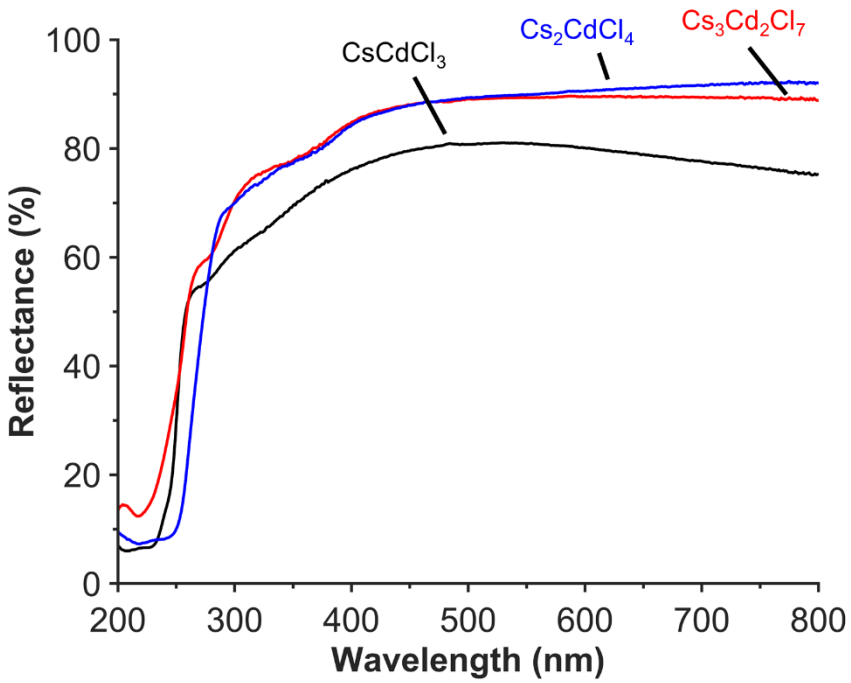


**Figure S6.** Diffuse reflectance spectrum from 200-800 nm for $CsCdCl_3$, $Cs_2CdCl_4$, and $Cs_3Cd_2Cl_7$ particles.

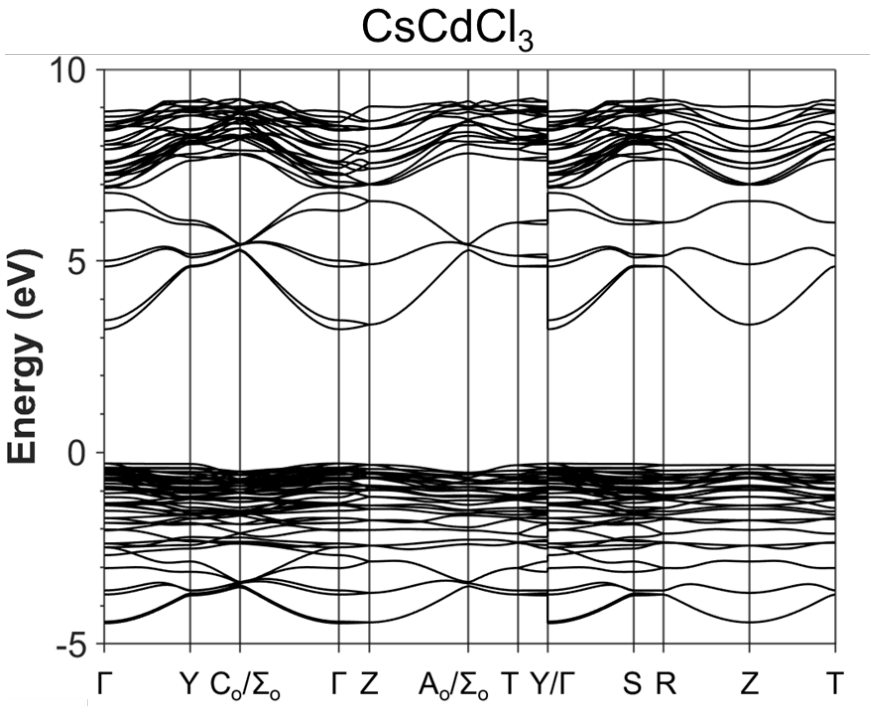


**Figure S7.** Calculated PBE band structure corrected using a scissor operator with the HSE band gap for $CsCdCl_3$.

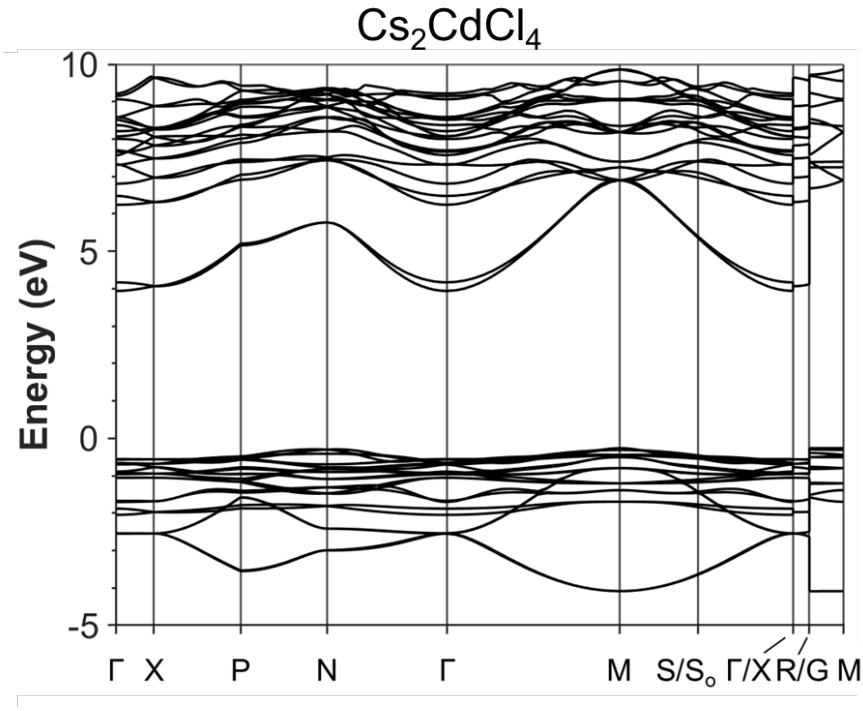


**Figure S8.** Calculated PBE band structure corrected using a scissor operator with the HSE band gap for $Cs_2CdCl_4$.

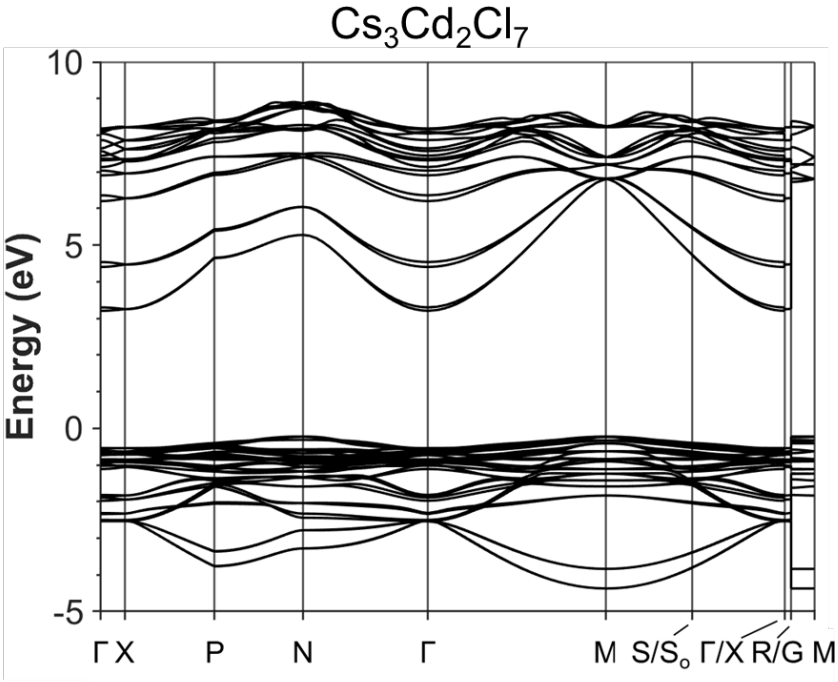


**Figure S9.** Calculated PBE band structure corrected using the scissor operator with the HSE band gap for $Cs_3Cd_2Cl_7$.

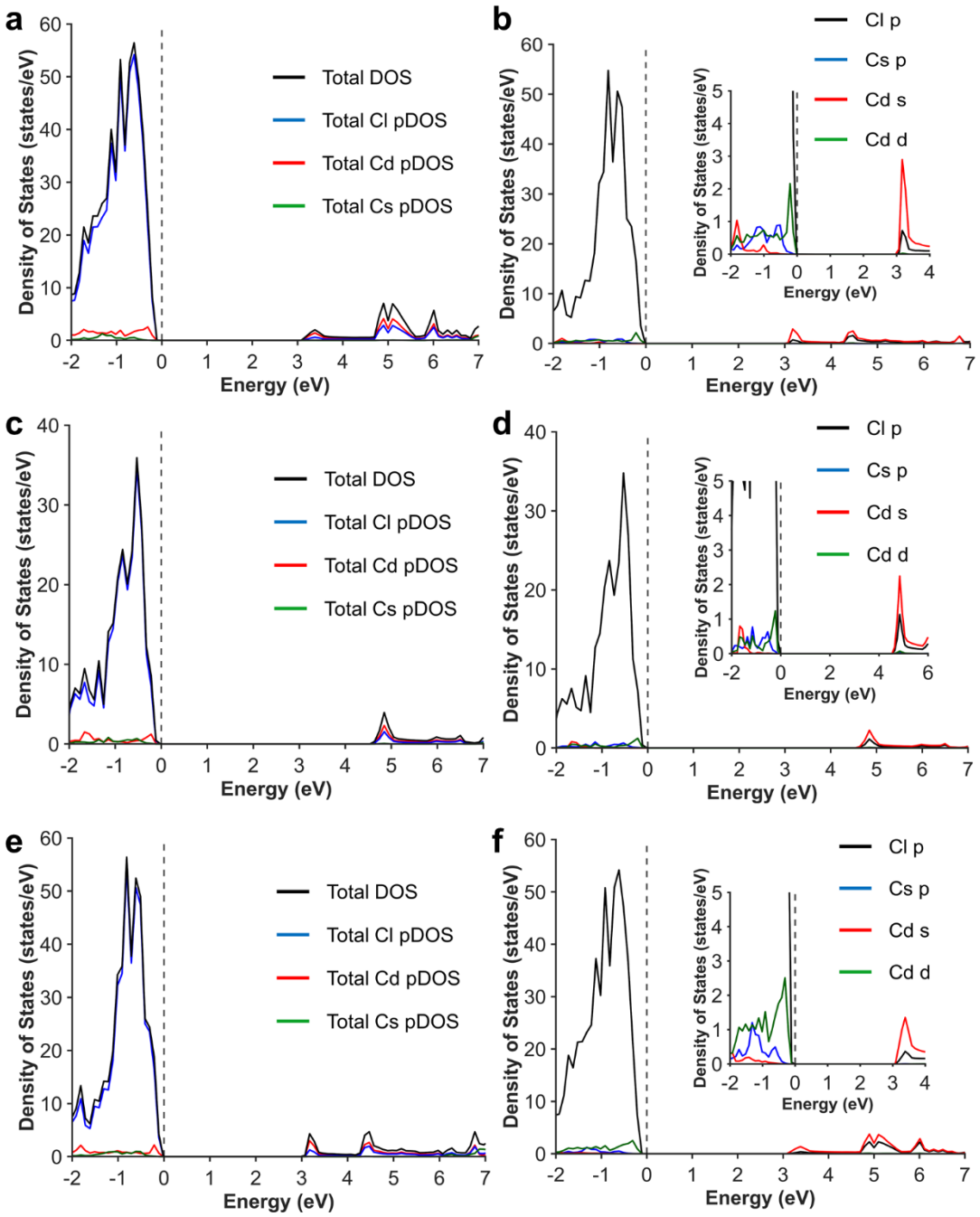


**Figure S10**. (a,c,e) Computed total density of states of Cl, Cd, and Cs for $CsCdCl_3$, $Cs_2CdCl_4$, and $Cs_3Cd_2Cl_7$, respectively. (b,d,f) Computed projected density of states for Cl p, Cs p, Cd s, and Cd d orbitals for $CsCdCl_3$, $Cs_2CdCl_4$, and $Cs_3Cd_2Cl_7$, respectively. The insets show magnified projected density of states in order to discern the Cs p, Cd d, and Cd s orbitals.