Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

ELECTRONIC SUPPLEMENTARY INFORMATION

On the missing links in quantum dot solar cells: A DFT study on fluorophore oxidation and reduction processes in sensitized solar cells

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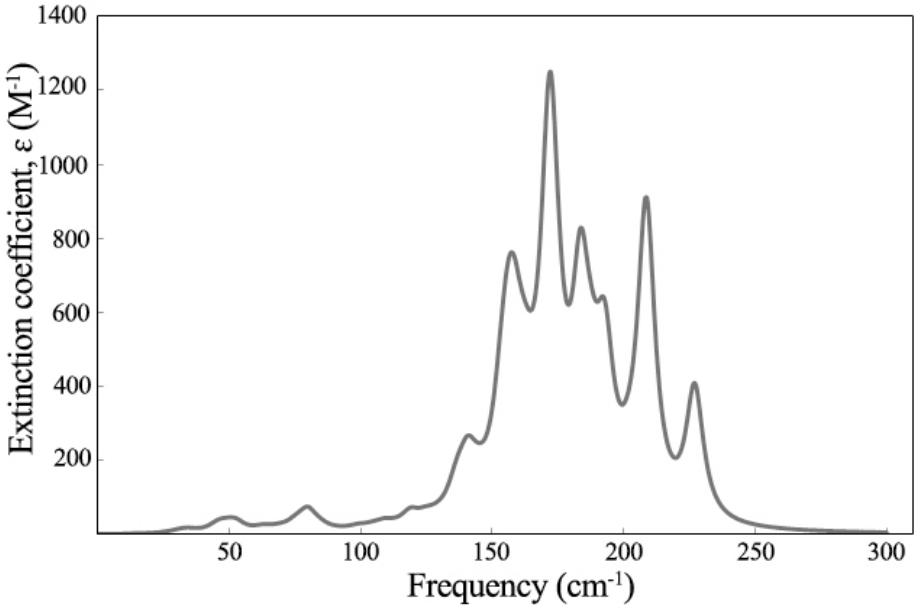
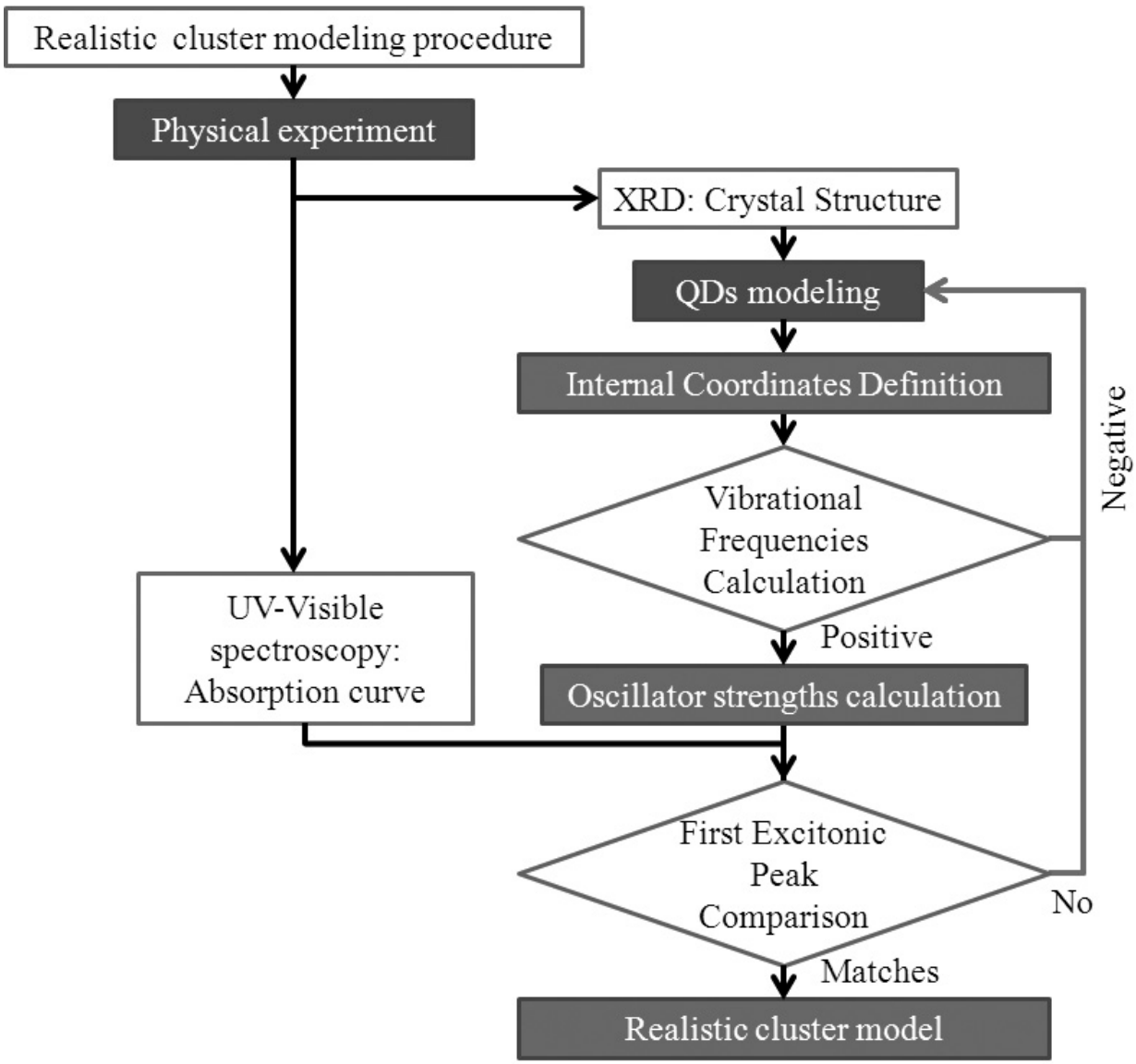
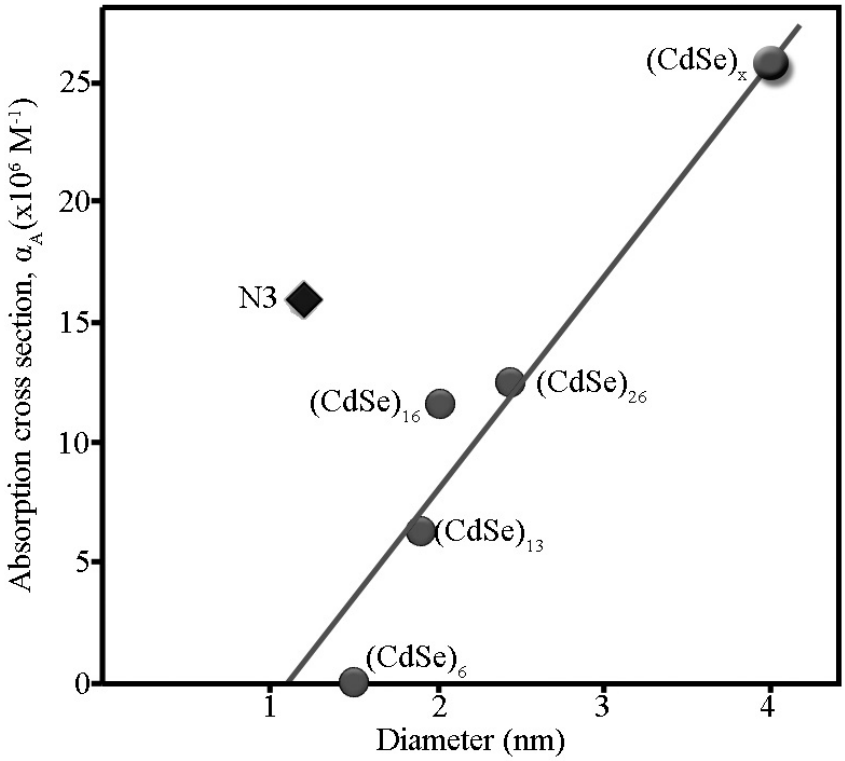


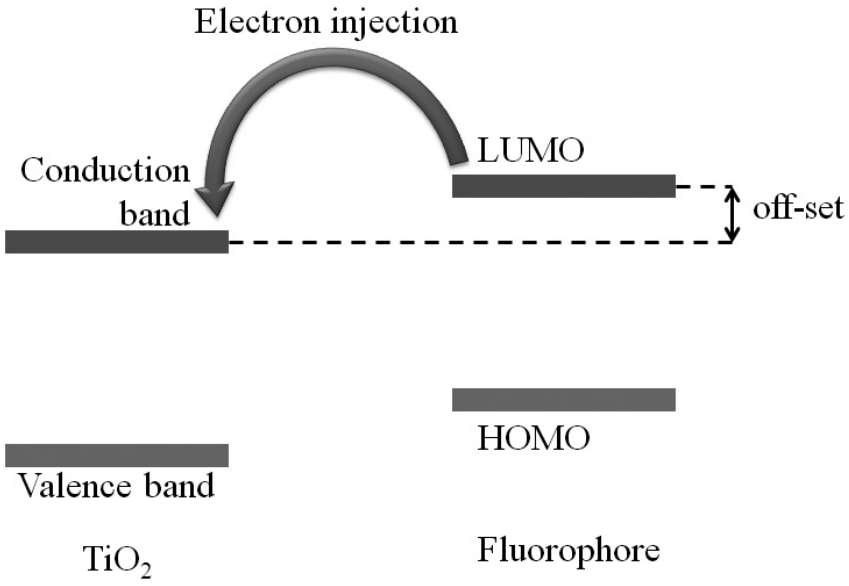
S1. Calculated Infrared spectra of $(CdSe)_{26}$ cluster shows positive frequencies confirming a minimum energy structure.



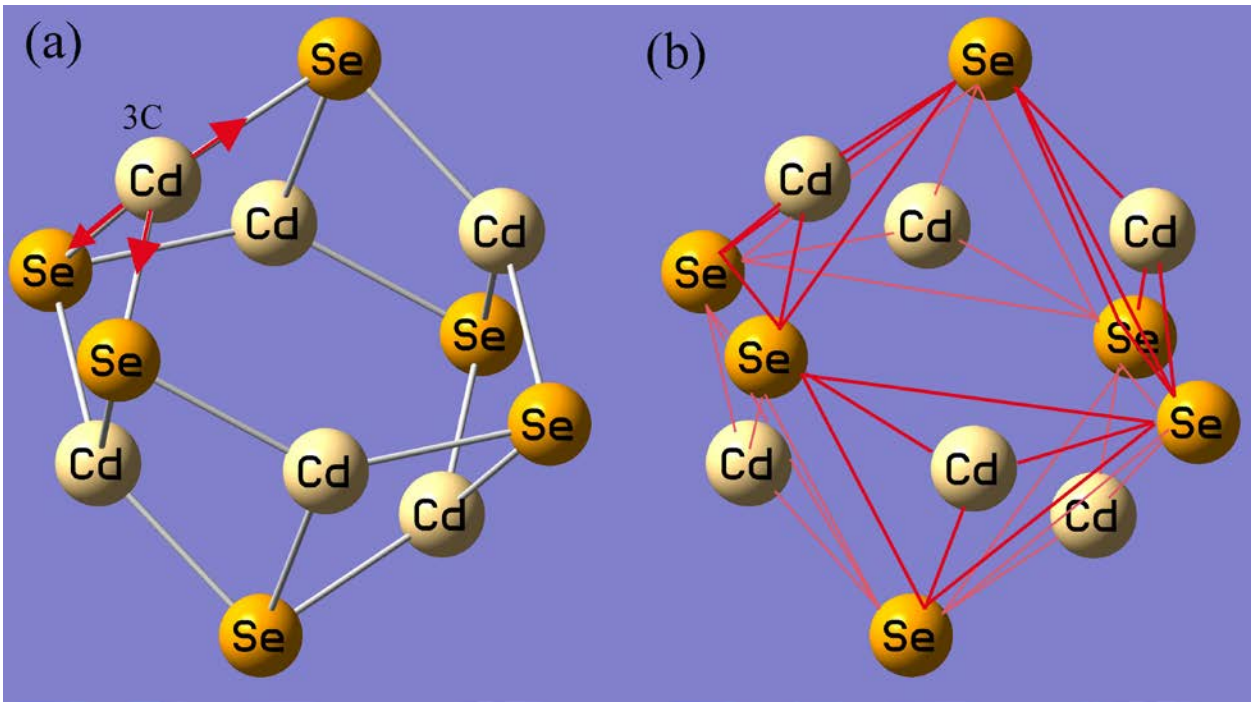
S2. Procedure of realistic cluster modeling.



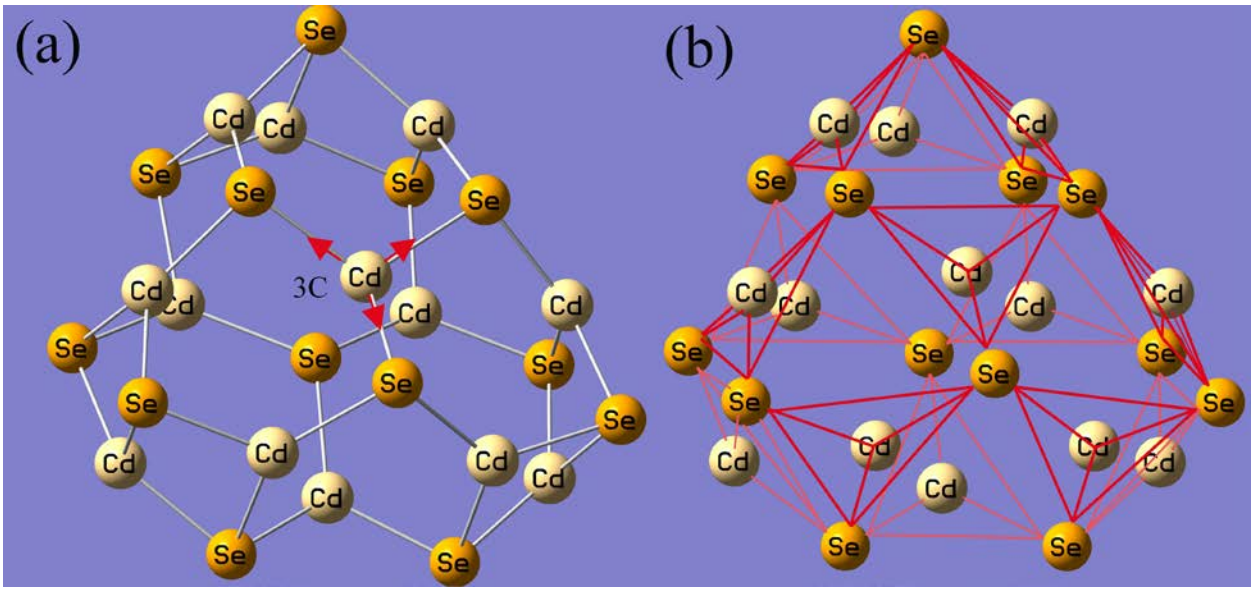
S3. Absorption cross section of $(CdSe)_x$ QDs with diameter of ~4 nm is predicted higher than that of N3 dye molecule.



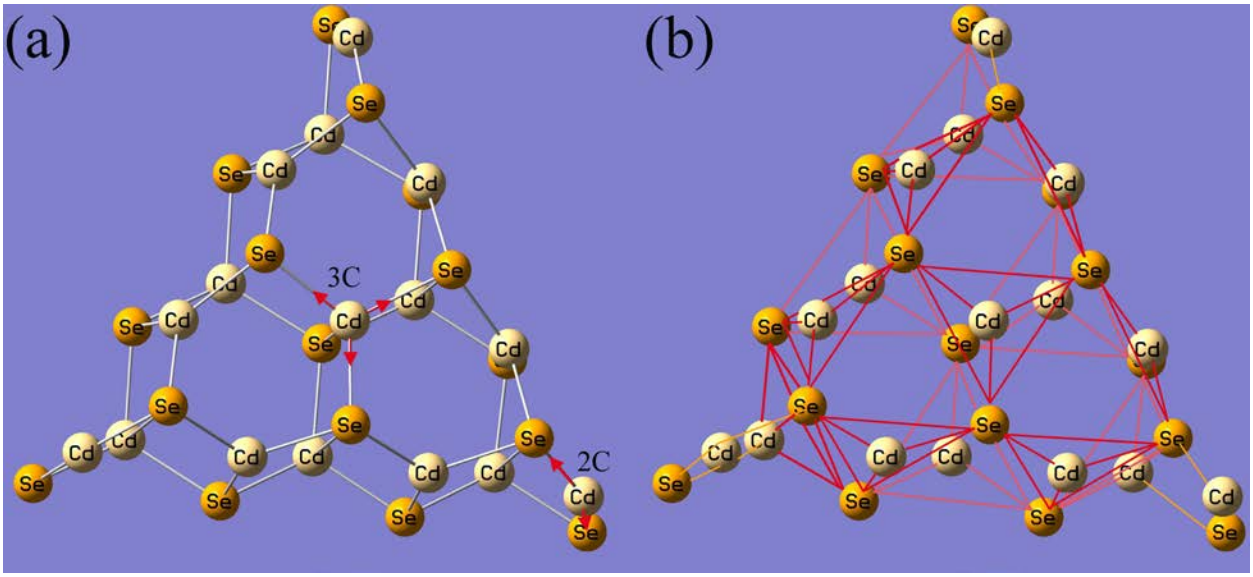
S4. Off-set minimization could minimize the amount of energy lost during injection and increase the final conversion efficiency.



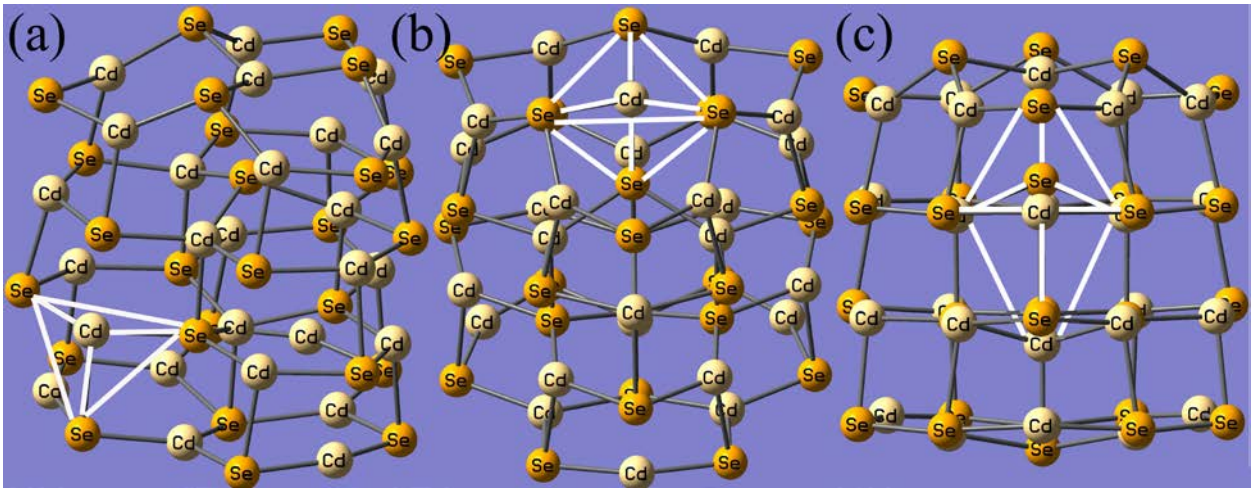
S5. (a) Optimized structure of $(CdSe)_6$ which contains 3C Cadmium atomic sites made by (b) stacking of 6 trigonal pyramids which also the surface atoms that involve in ligand adsorption.



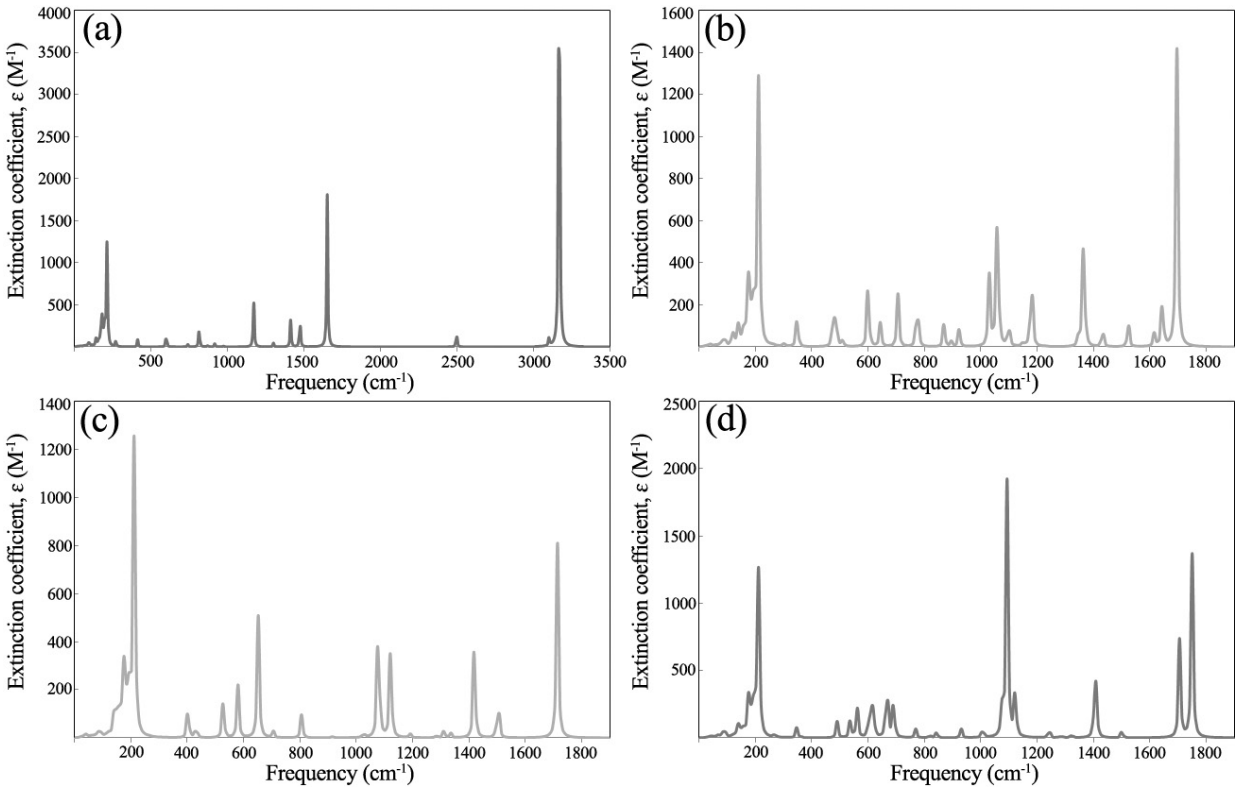
S6. (a) Optimized structure of $(CdSe)_{13}$ which contains 3C Cadmium atomic sites made by (b) stacking of 13 trigonal pyramids which also the surface atoms that involve in ligand adsorption.



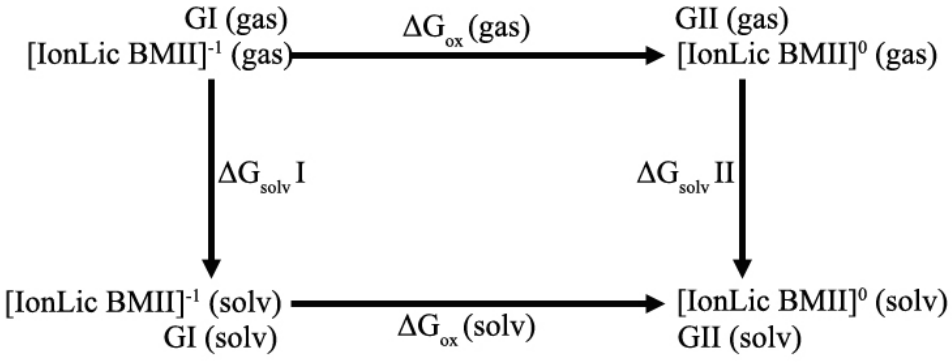
S7. (a) Optimized structure of $(CdSe)_{16}$ which contains 2C and 3C Cadmium atomic sites made by (b) stacking of 13 trigonal pyramids which also the surface atoms that involve in ligand adsorption.



S8. Cluster of $(CdSe)_{26}$ which contains (a) surface 3C (trigonal pyramid) Cadmium atomic sites that involve in ligand adsorption, (b) interior 4C (tetrahedron) and (c) interior 5C (trigonal bipyramid) Cadmium atomic sites that do not involve in ligand adsorption.



S9. Calculated Infrared spectra of (a) $(CdSe)_{13}$–MAA, (b) $(CdSe)_{13}$–MBA , (c) $(CdSe)_{13}$–MPA and (d) $(CdSe)_{13}$–MSA conjugates show positive frequencies confirming minimum energy structures.



S10. Born-Haber thermodynamic cycle for standard redox potential calculations.