Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supporting Information

Highly Qualified InP Based QDs via Temperature Controlled ZnSe Shell Coating Process and Their DFT Calculation

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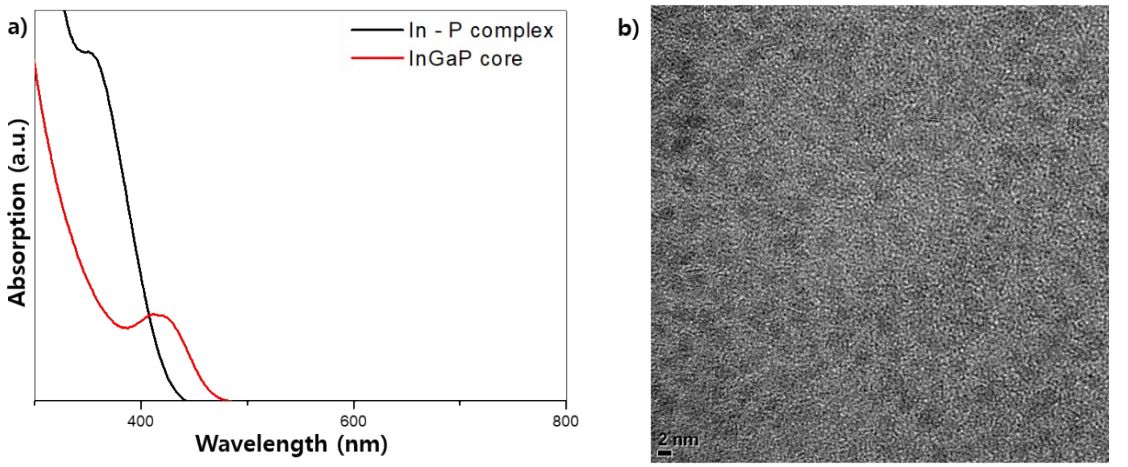

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igure S1. a) Absorption spectrum data of In-P complex(black line) and InGaP core(red line), b) TEM image of InGaP core.

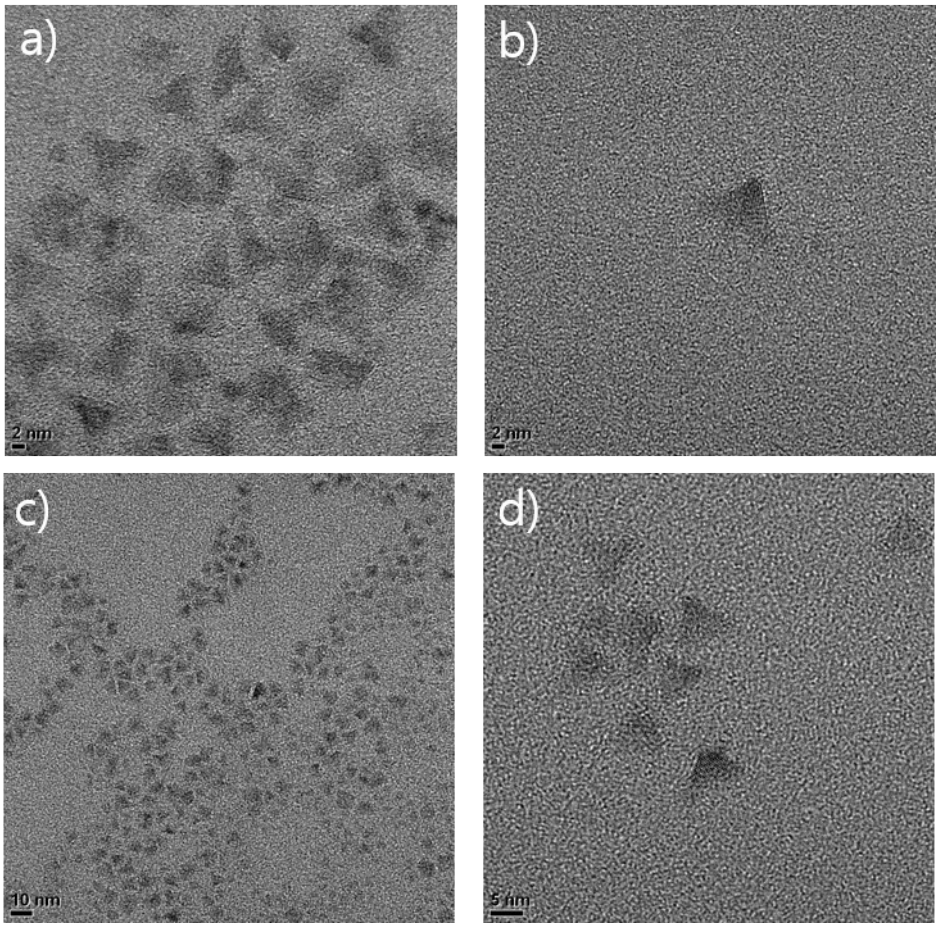

Figure S2. a-d) TEM image of InGaP/ZnSe/ZnS QDs of 320 °C ZnSe shell coated.

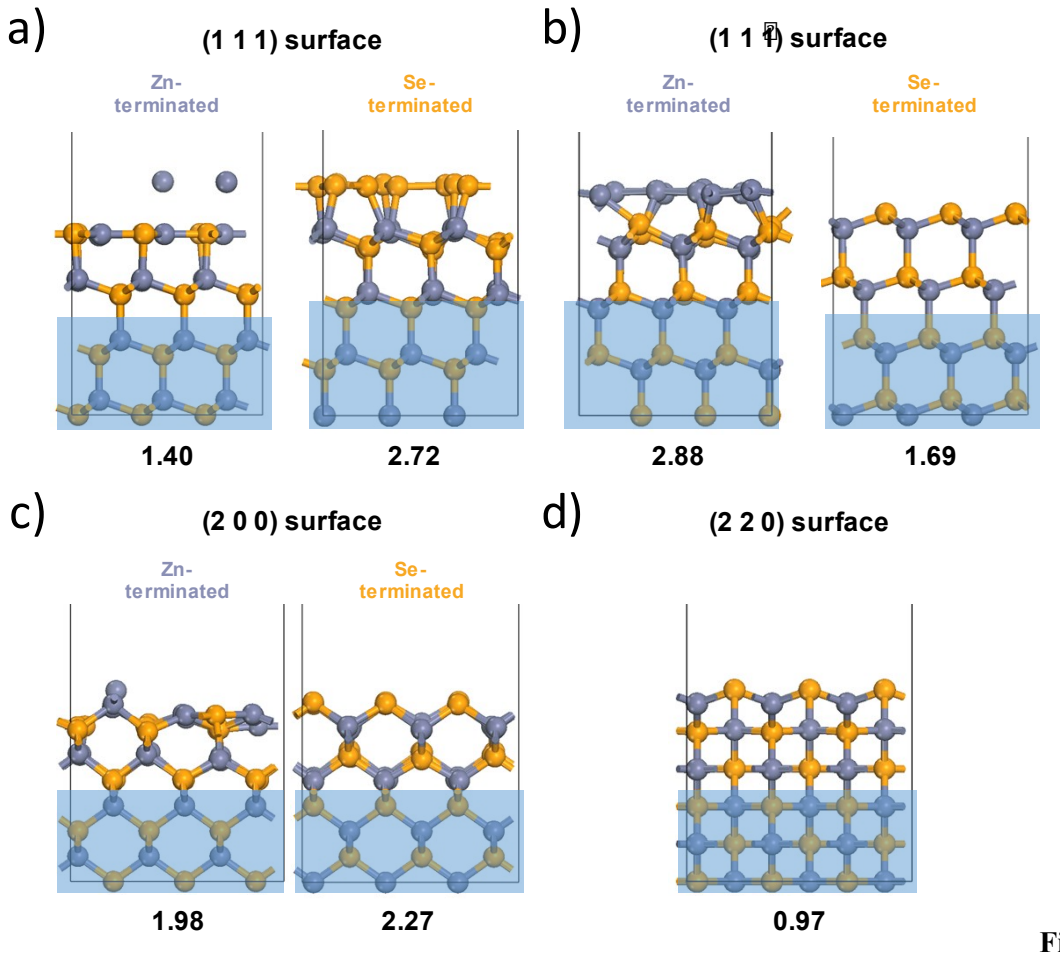

Figure S3. Optimized slab models of a) ZnSe (111) surface, b) (11$\bar{1}$) surface, c) (200) surface, and d) (220) surface. (111) surface, (11$\bar{1}$) surface, and (200) surface are the polar surfaces which have two different kinds of termination; Zn- and Se-termination. (220) surface is the non-polar surface. The numbers below each figure represent the surface energy (in kcal/mol/Å^2). The bottom blue regions were fixed to theoretically mimic the bulk phase. Zn and Se are represented by navy and orange colored spheres, respectively.

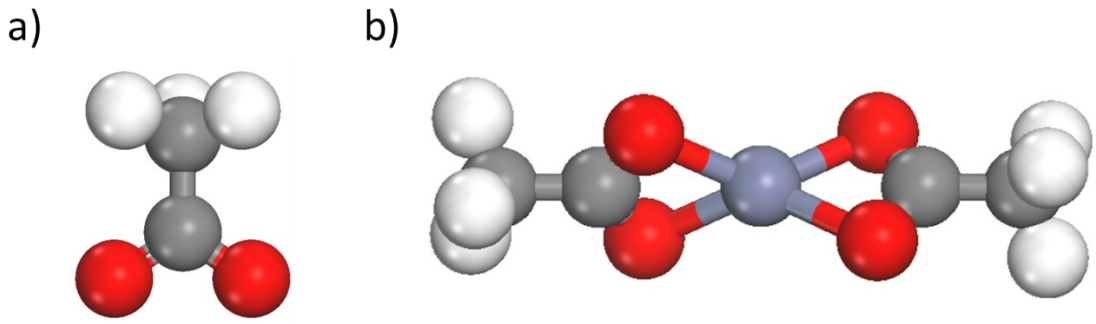

Figure S4. Optimized ligand models of a) oleate, b) $Zn(oleate)_2$. The acetate ion was used to represent the oleate ion, which have the same carboxylate group.[S1-S4] Zn, O, C, and H are represented by navy, red, grey and white colored spheres, respectively.

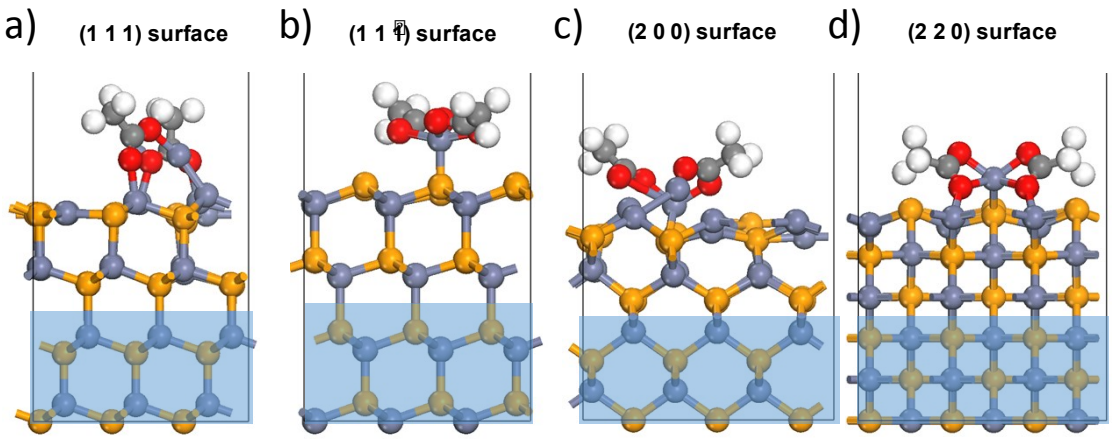

Figure S5. Optimized structures of each ZnSe surface with $Zn(oleate)_2$ model; a) ZnSe (111) surface, b) $(11\bar{1})$ surface, c) (200) surface, and d) (220) surface. The bottom blue regions were fixed to theoretically mimic the bulk phase. Zn, Se, O, C, and H are represented by navy, orange, red, grey and white colored spheres, respectively.

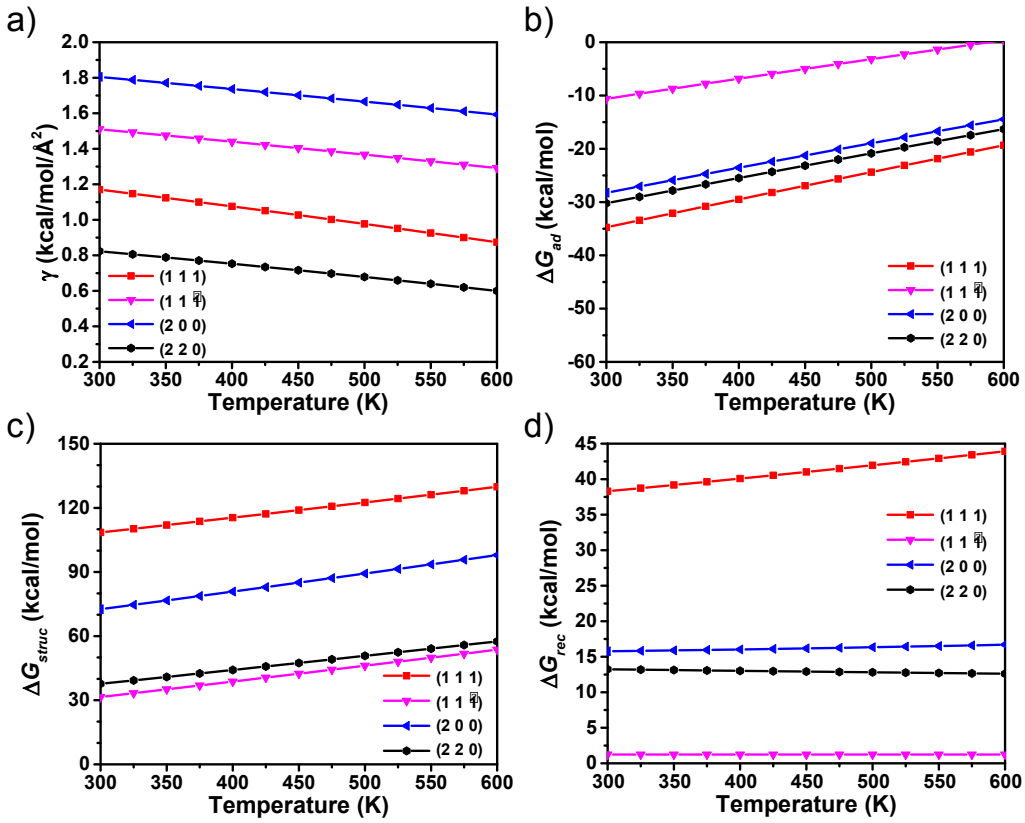

Figure S6. a) Surface free energy (γ), b) Gibbs free energy for adsorption of oleate (ΔG_{ad}) to each ZnSe surface, c) Gibbs free energy for structural change of adsorbed Zn(oleate)$_2$ (ΔG_{struc}), and d) Gibbs free energy for reconstruction of surface (ΔG_{rec}) as a function of the temperature. Note that γ is calculated by Eq.(7), ΔG_{ad} is calculated by Eqs.(1) and (3), ΔG_{struc} is calculated by Eqs.(1) and (5), and ΔG_{rec} is calculated by Eqs.(1) and (4).

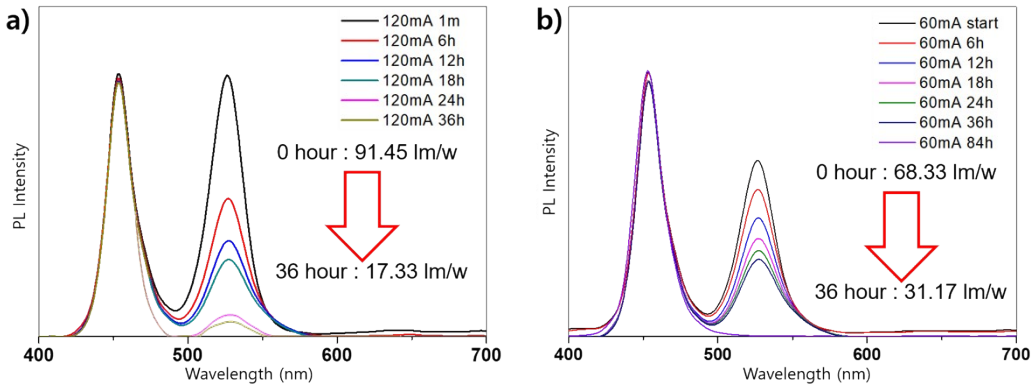

Figure S7. Temporal change of on-chip LED spectra of green-light emitting InP with POSS resin at a) 10V-120 mA, b) 10V-60 mA.

Table S1. Interplanar distance according to the miller indices of the possible growth surfaces of zinc-blende ZnSe

h k l	**Interplanar distance (Å)**
{111}	3.272
$\{11\bar{1}\}$	3.272
{200}	2.834
{220}	2.004

Table S2. Lattice parameters *a, b*, and φ for the slab models and coverage (θ) of $Zn(oleate)_2$ to each surface for used in the calculation for the relaxed surface free energy. θ was assumed to be equal to the number of dangling Se on each surface divided by twice of area. Since the ligand consists of two oleate ions, the coverage for ligand adsorption was taken to be a half of the number of dangling atoms exposed on each surface.

h k l	***a* (Å)**	***b* (Å)**	**φ (°)**	**θ ($Zn(oleate)_2$/Å²)**
{111}	12.0137	12.0137	120	0.036
$\{11\bar{1}\}$	12.0137	12.0137	120	0.036
{200}	12.0137	12.0137	90	0.022
{220}	11.3266	12.0137	90	0.031

References

S1. P. R. McGill, and H. Idriss, *Surf. Sci.* 2008, **602**, 3688-3695.
S2. E. Hwang, D. H. Kim, Y. J. Hwang, A. Kim, S. Hong, and S. Kim, *J. Phys. Chem. C* 2007, **111**, 5941-5945.
S3. L. Liu, Z. Zhuang, T. Xie, Y.-G. Wang, J. Li, Q. Peng, and Y. Li, *J. Am. Chem. Soc.* 2009, **131**, 16423–16429.
S4. O. Voznyy, *J. Phys. Chem. C* 2011, **115**, 15927–15932.