Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY DATA

TABLE S1. The layer thickness (d), angles (Θ_1, Θ_2, Θ_3, Θ_4) of relaxed and strain structures**.**

Strain	**d(Å)**	**Θ_1(°)**	**Θ_2(°)**	**Θ_3(°)**	**Θ_4(°)**
Relaxed	3.14	91.15	88.86	90.88	89.09
ε_x= 6%	3.08 (-1.91%)	91.54 (-0.43%)	88.57 (-0.33%)	89.08 (-1.98%)	93.96 (5.47%)
ε_y= 8%	3.06 (-2.54%)	86.47 (-4.68%)	93.48 (5.20%)	93.54 (2.93%)	86.21 (-3.23%)

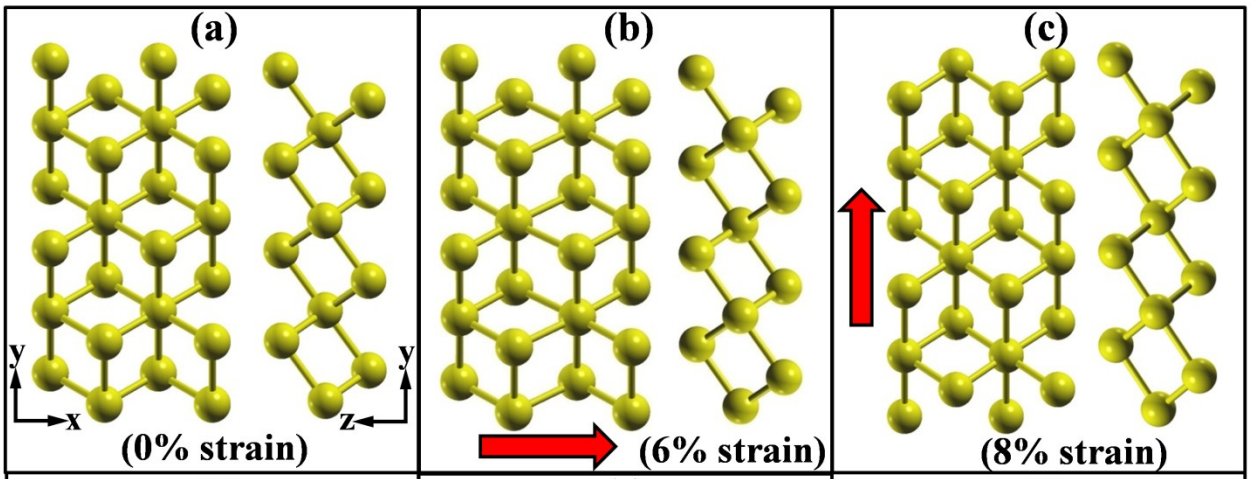


Figure S1. Structural variation with respect to strain **(a), (b), (c)** Structures of α-Se at 0%, 6% (along x-direction), 8% (along y-direction) strain.

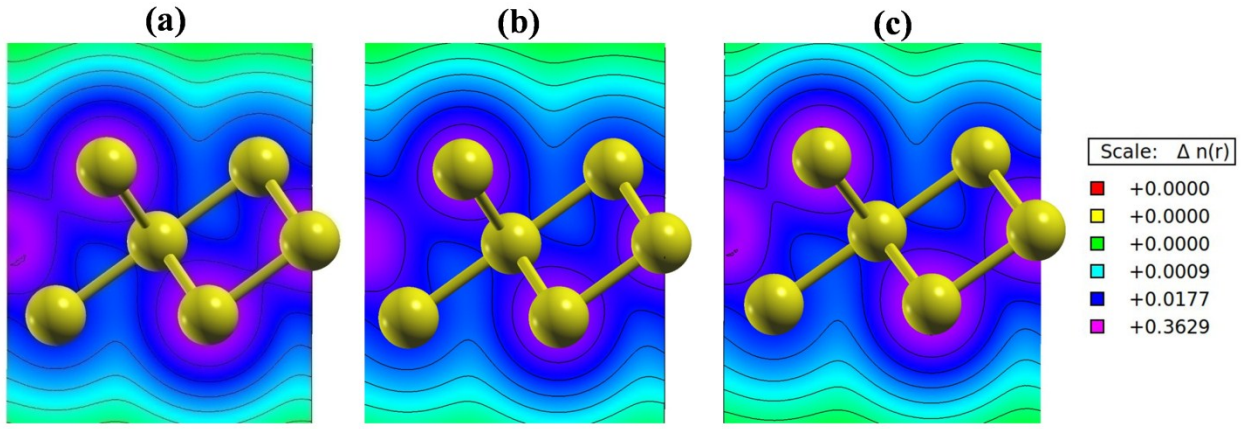
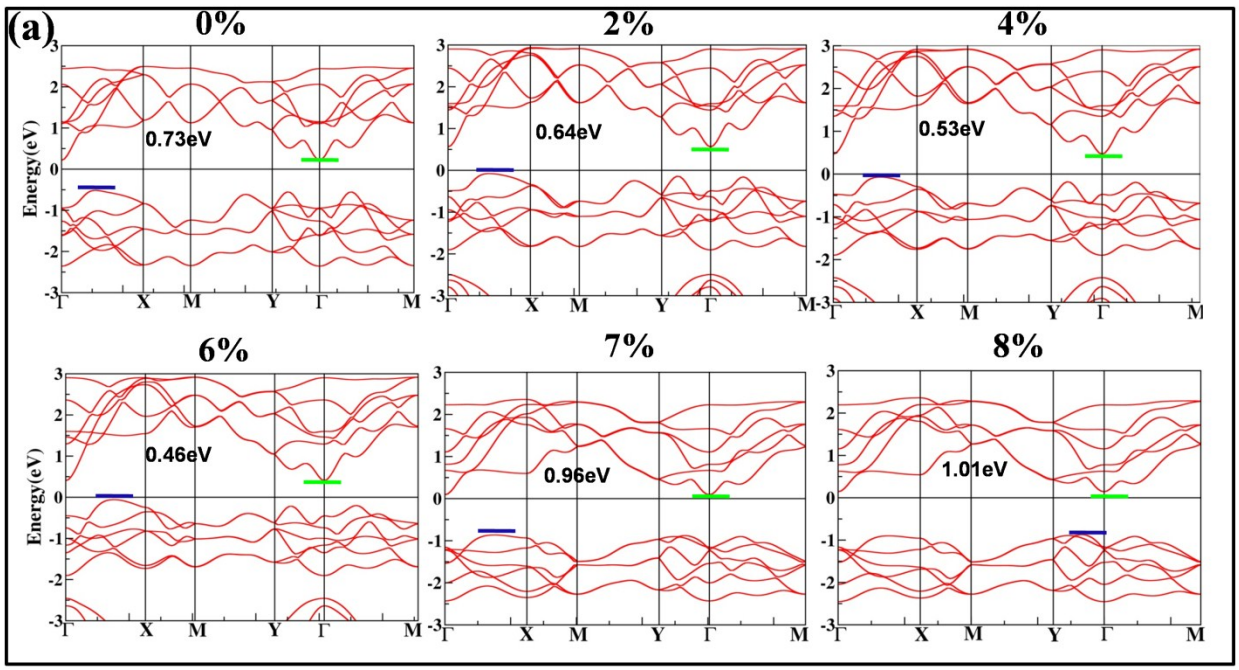


Figure S2. Charge density profile of α-Se (a) at 0%, (b) at 6% (along x-direction), (c) 6% (along y-direction) strain.



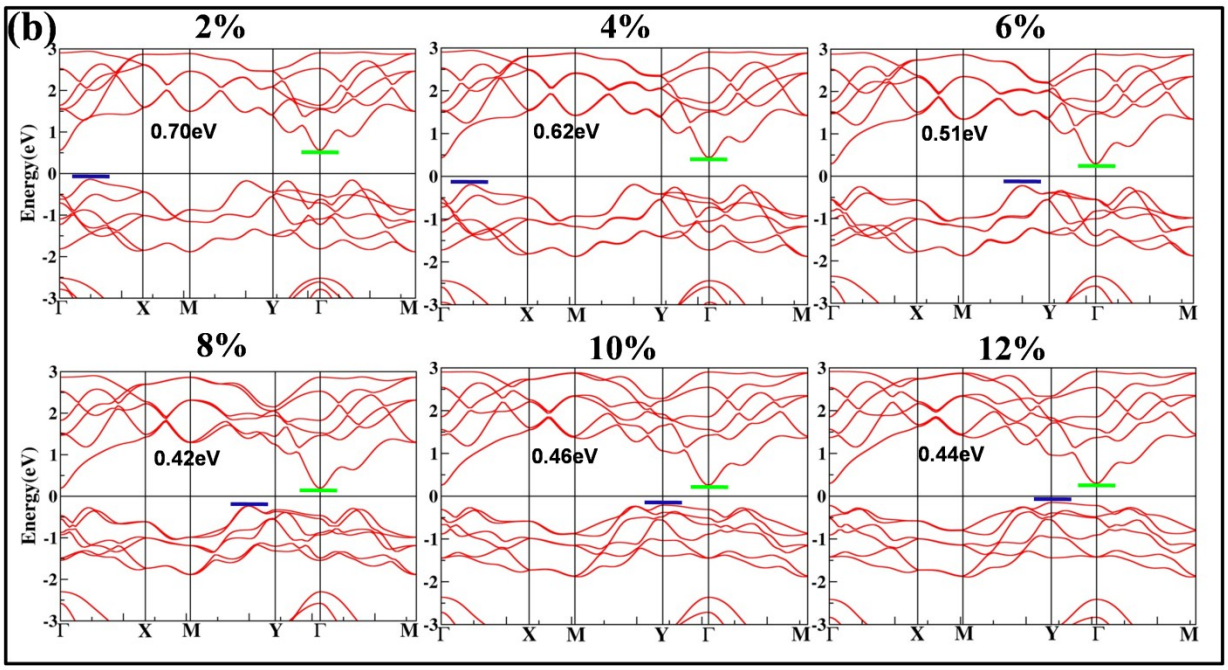


Figure S3. Effect of strain on band structures of α-Se. **(a)** Along X-direction (6% is the critical strain). **(b)** Along Y-direction (8% is the critical strain)..

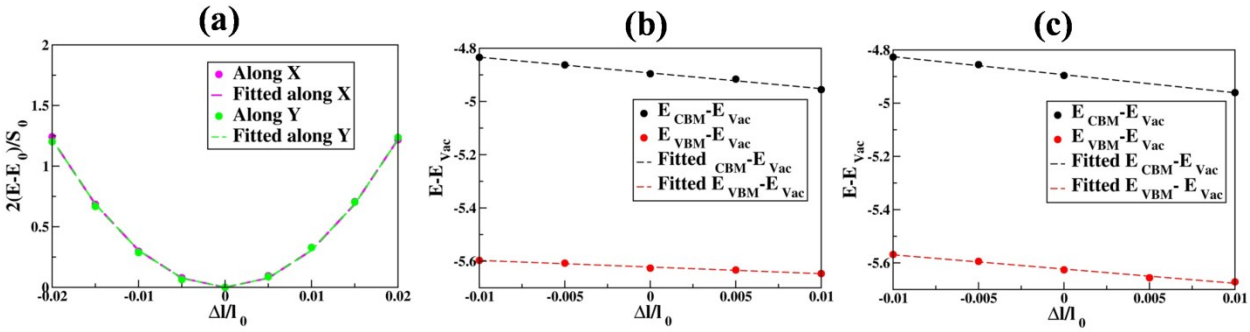


Figure S4. (a) Graph and parabolic fit between $\frac{2(E-E_0)}{S_0}$ and $\frac{\Delta l}{l_0}$, $E-E_0$ is the difference in the total energy of stable and strained structure, S_0 is the surface area of monolayer slab of α-Se and $\frac{\Delta l}{l_0}$ is the strain in the corresponding direction. **(b), (c)** Graph and straight fit graph between

$E - E_{vac}$ and $\frac{\Delta l}{l_0}$ along x and y direction, $E - E_{vac}$ is the difference in the energy of ith band and vacuum energy, $\frac{\Delta l}{l_0}$ is the strain in the corresponding direction.