# Supporting information for

## Electronic, mechanical and gas sensing properties of two-dimensional γ-SnSe

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**Table S1**. The optimized structural parameters of monolayer and multilayer γ-SnSe.

| Model | $a$ (Å) | $b$ (Å) | $c$ (Å) (includes vacuum layer thickness) |
|---|---|---|---|
| Monolayer | 3.906 | 6.207 | 22.417 |
| Bilayer | 3.998 | 6.202 | 26.594 |
| Trilayer | 4.041 | 6.195 | 30.771 |
| Four-layer | 4.068 | 6.190 | 34.948 |
| Five-layer | 4.085 | 6.187 | 39.125 |

**Table S2**. The corresponding bond angles of optimized monolayer and multilayer γ-SnSe.

| Model | layer | $\theta_1$ (°) | $\theta_2$ (°) | $\theta_3$ (°) | $\theta_4$ (°) | $\theta_5$ (°) |
|---|---|---|---|---|---|---|
| Monolayer | 1 | 91.347 | 98.003 | 91.014 | 91.347 | 91.014 |
| Bilayer | 2-1 | 91.605 | 100.487 | 92.824 | 90.004 | 92.969 |
| | 2-2 | 91.605 | 100.487 | 92.824 | 90.004 | 92.969 |
| Tri-layer | 3-1 | 91.852 | 100.530 | 93.554 | 89.751 | 93.789 |
| | 3-2 | 90.513 | 102.638 | 93.330 | 90.513 | 93.330 |
| | 3-3 | 89.751 | 102.556 | 93.789 | 91.852 | 93.554 |
| Four-layer | 4-1 | 91.913 | 100.600 | 94.077 | 89.601 | 94.344 |
| | 4-2 | 90.194 | 103.265 | 93.601 | 90.590 | 93.502 |
| | 4-3 | 90.194 | 103.265 | 93.601 | 90.590 | 93.502 |
| | 4-4 | 91.913 | 100.600 | 94.077 | 89.601 | 94.344 |
| Five-layer | 5-1 | 91.944 | 100.594 | 94.420 | 89.587 | 94.715 |
| | 5-2 | 89.976 | 103.508 | 93.822 | 90.667 | 93.729 |
| | 5-3 | 90.202 | 103.510 | 93.499 | 90.202 | 93.499 |
| | 5-4 | 90.667 | 102.850 | 93.729 | 89.976 | 93.822 |
| | 5-5 | 89.587 | 102.859 | 94.715 | 91.944 | 94.420 |

**Table S3**. The corresponding bond lengths and the interlayer distances of optimized monolayer and multilayer γ-SnSe.

| Model | layer | $l_1$ (Å) | $l_2$ (Å) | $l_3$ (Å) | $l_4$ (Å) | $d$ (Å) |
|---|---|---|---|---|---|---|
| Monolayer | 1 | 2.738 | 2.890 | 2.738 | 2.890 | / |
| Bilayer | 2-1 | 2.756 | 2.814 | 2.760 | 2.857 | / |
| | 2-2 | 2.756 | 2.814 | 2.760 | 2.857 | 2.159 |
| Trilayer | 3-1 | 2.767 | 2.799 | 2.773 | 2.851 | / |
| | 3-2 | 2.778 | 2.811 | 2.778 | 2.811 | 2.058 |
| | 3-3 | 2.773 | 2.851 | 2.767 | 2.799 | 2.058 |
| Four-layer | 4-1 | 2.773 | 2.791 | 2.779 | 2.849 | / |
| | 4-2 | 2.792 | 2.806 | 2.790 | 2.799 | 2.017 |
| | 4-3 | 2.792 | 2.806 | 2.790 | 2.799 | 1.943 |
| | 4-4 | 2.773 | 2.791 | 2.779 | 2.849 | 2.017 |
| Five-layer | 5-1 | 2.777 | 2.790 | 2.783 | 2.847 | / |
| | 5-2 | 2.799 | 2.808 | 2.797 | 2.794 | 1.996 |
| | 5-3 | 2.804 | 2.797 | 2.804 | 2.797 | 1.897 |
| | 5-4 | 2.797 | 2.794 | 2.799 | 2.808 | 1.897 |
| | 5-5 | 2.783 | 2.847 | 2.777 | 2.790 | 1.996 |

**Table S4**. The independent elastic constants $C_{11}$, $C_{22}$, $C_{12}$, $C_{66}$ of monolayer and multilayer γ-SnSe.

| Model | $C_{11}$ | $C_{22}$ | $C_{12}$ | $C_{66}$ |
|---|---|---|---|---|
| Monolayer | 24.329 | 25.729 | -0.598 | 6.161 |
| Bilayer | 39.512 | 47.117 | 3.201 | 15.736 |
| Tri-layer | 53.831 | 72.170 | 5.678 | 25.036 |
| Four-layer | 69.040 | 100.287 | 9.003 | 34.791 |
| Five-layer | 88.137 | 129.780 | 11.182 | 45.371 |

**Table S5**. The maximum and minimum Young's modulus (N m$^{-1}$) and Poisson's ratios of monolayer and multilayer γ-SnSe.

| Model | $Y_{max}$ | $Y_{min}$ | $v_{max}$ | $v_{min}$ |
|---|---|---|---|---|
| Monolayer | 25.715 | 16.377 | 0.329 | -0.025 |
| Bilayer | 46.858 | 36.986 | 0.190 | 0.068 |
| Tri-layer | 71.571 | 53.384 | 0.148 | 0.079 |
| Four-layer | 99.113 | 68.232 | 0.137 | 0.090 |
| Five-layer | 128.361 | 87.173 | 0.129 | 0.086 |
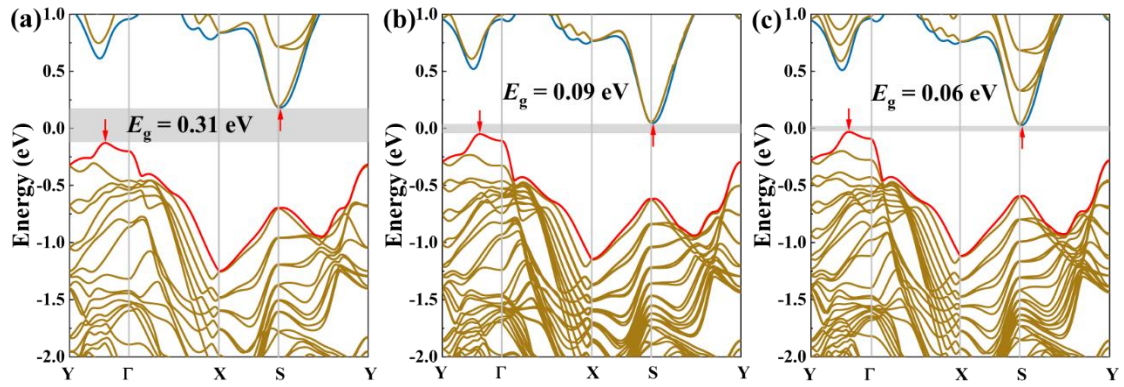


**Figure S1.** Electronic band structure of (a) six-layer, (b) nine-layer and (c) ten-layer γ-SnSe based on PBE+SOC calculation.
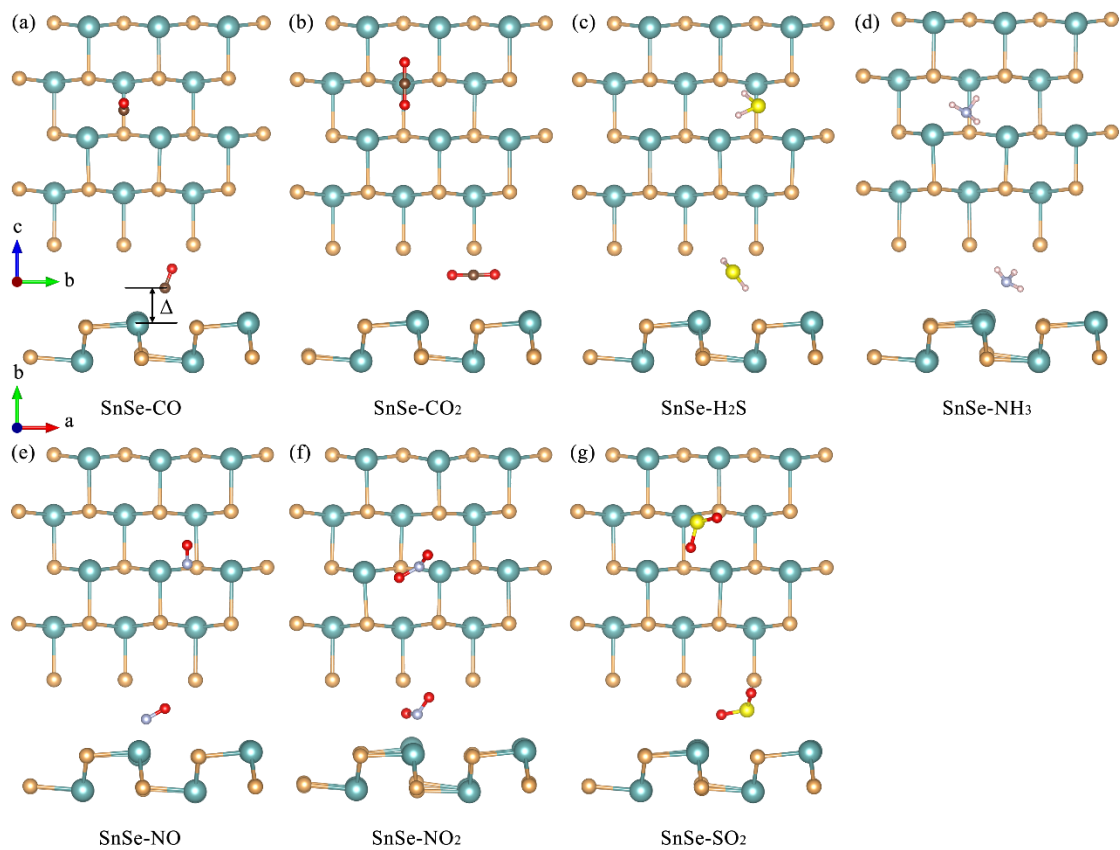
**Figure S2**. The most stable configurations of gas molecules (CO, $CO_2$, $H_2S$, $NH_3$, NO, $NO_2$, and $SO_2$) adsorbed on the ML $\gamma$-SnSe.