Supplementary Information

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| B1 | B2 | B3 | B4 | H1 | H2 | H3 |
| H4 | TM1 | TM2 | TM3 | TS1 | TS2 | TS3 |

**Fig. S1** Initial configurations for the adsorption of $\text{H}_2\text{S}$ molecule above the SL-MoS$_2$ surface. Purple (yellow) atoms represent Molybdenum (Sulfur).
Table S1 Zero-crossing energies for the real part of the dielectric function spectra ($\varepsilon_1$) for pristine and H$_2$S adsorbed SL-MoS$_2$ under different strains and concentrations of gas molecules.

| System     | Strain (%) | Num. of H$_2$S Mol. | 1st    | 2nd    | 3rd    | 4th    | 5th    | 6th    | 7th    | 8th    | 9th    | 10th   |
|------------|------------|---------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| SL-MoS$_2$ | -8         | None                | 4.641  | 6.591  | 7.384  | 8.321  | 12.33  | 13.11  | 15.32  | -      | -      | -      |        |
|            | -8         | 1                   | 4.608  | 6.555  | 7.361  | 12.34  | 13.18  | 15.36  | 16.36  | -      | -      | -      |        |
|            | -8         | 2                   | 4.585  | 6.524  | 7.342  | 12.36  | 13.26  | 15.4   | 16.41  | -      | -      | -      |        |
|            | -8         | 3                   | 4.565  | 6.489  | 7.323  | 12.39  | 13.3   | 15.48  | 16.5   | -      | -      | -      |        |
|            | -8         | 4                   | 4.525  | 6.34   | 7.325  | 12.37  | 13.41  | 15.54  | 16.49  | -      | -      | -      |        |
|            | -6         | None                | 4.657  | 7.298  | 7.59   | 8.181  | 12.99  | 13.73  | 15.11  | 15.98  | -      | -      |        |
|            | -6         | 1                   | 4.642  | 6.493  | 7.274  | 8.08   | 13.01  | 13.71  | 15.17  | 16.03  | -      | -      |        |
|            | -6         | 2                   | 4.629  | 6.45   | 7.248  | 13.06  | 15.24  | 16.13  | -      | -      | -      | -      |        |
|            | -6         | 3                   | 4.622  | 6.409  | 7.212  | 13.09  | 16.35  | -      | -      | -      | -      | -      |        |
|            | -6         | 4                   | 4.539  | 6.292  | 7.229  | 8.112  | 12.22  | 13.1   | 16.34  | -      | -      | -      |        |
|            | -4         | None                | 4.693  | 7.238  | 8.059  | 12.83  | 13.74  | 14.44  | 14.94  | 15.56  | -      | -      |        |
|            | -4         | 1                   | 4.682  | 7.216  | 7.987  | 12.85  | 13.75  | 14.53  | 14.99  | 15.68  | -      | -      |        |
|            | -4         | 2                   | 4.664  | 7.193  | 7.849  | 12.87  | 13.76  | 16.02  | -      | -      | -      | -      |        |
|            | -4         | 3                   | 4.645  | 7.167  | 12.91  | 16.11  | -      | -      | -      | -      | -      | -      |        |
|            | -4         | 4                   | 4.605  | 6.193  | 7.177  | 8.12   | 12.93  | 16.11  | -      | -      | -      | -      |        |
|            | -2         | None                | 4.665  | 7.138  | 8.276  | 13.72  | 14.4  | 14.83  | 15.47  | -      | -      | -      |        |
|            | -2         | 1                   | 4.652  | 7.127  | 7.821  | 8.238  | 13.76  | 14.47  | 14.86  | 15.55  | -      | -      |        |
|            | -2         | 2                   | 4.643  | 7.114  | 7.696  | 8.194  | 14.53  | 14.9  | 15.68  | -      | -      | -      |        |
|            | -2         | 3                   | 4.629  | 7.101  | 7.542  | 7.565  | 7.581  | 15.79  | -      | -      | -      | -      |        |
|            | -2         | 4                   | 4.586  | 6.093  | 7.109  | 7.507  | 8.24   | 15.87  | -      | -      | -      | -      |        |
| SL-MoS$_2$ | 0          | None                | 3.06   | 4.516  | 5.438  | 7.058  | 7.542  | 8.07   | 14.15  | 15.45  | -      | -      |        |
|            | 2          | None                | 3.009  | 4.517  | 5.434  | 7.037  | 7.469  | 7.991  | 14.33  | 15.37  | -      | -      |        |
|            | 4          | None                | 3.005  | 5.372  | 6.97   | 7.966  | 13.99  | 15.23  | -      | -      | -      | -      |        |
|            | 6          | None                | 2.941  | 5.339  | 6.74   | 6.96   | 7.682  | 11.9   | 14.08  | 14.39  | 15.2   | -      |        |
|            | 8          | None                | 2.532  | 5.364  | 7.212  | -      | -      | -      | -      | -      | -      | -      |        |
|            | 2          | None                | 2.839  | 5.309  | 5.816  | 6.69   | 7.687  | 13.84  | -      | -      | -      | -      |        |
|            | 4          | None                | 2.835  | 5.305  | 5.816  | 6.655  | 7.662  | 13.86  | -      | -      | -      | -      |        |
|            | 6          | None                | 2.685  | 5.152  | 5.559  | 6.539  | 7.508  | 13.65  | -      | -      | -      | -      |        |
|            | 8          | None                | 2.526  | 5.366  | 7.237  | 14.11  | -      | -      | -      | -      | -      | -      |        |
| System | Strain (%) | Num. of H₂S Mol | 1st | 2nd | 3rd | 4th | 5th | 6th | 7th | 8th | 9th | 10th |
|--------|------------|----------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
|         | -8         |                |     |     |     |     |     |     |     |     |     |      |
| SL-MoS₂ |            |                |     |     |     |     |     |     |     |     |     |      |
| 1       | 0          |                |     |     |     |     |     |     |     |     |     |      |
|         | -2         |                |     |     |     |     |     |     |     |     |     |      |
|         | -4         |                |     |     |     |     |     |     |     |     |     |      |
|         | -6         |                |     |     |     |     |     |     |     |     |     |      |
|         | -8         |                |     |     |     |     |     |     |     |     |     |      |
|         | -10        |                |     |     |     |     |     |     |     |     |     |      |

Table S2: Energies and (relative) intensities of the first ten peaks in the EEL spectra for different strains and concentrations of H₂S molecules introduced to SL-MoS₂ sheet.